
DICE Embeddings

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Contents:

1 Dicee Manual	2
2 Installation	3
2.1 Installation from Source	3
3 Download Knowledge Graphs	3
4 Knowledge Graph Embedding Models	3
5 How to Train	3
6 Creating an Embedding Vector Database	5
6.1 Learning Embeddings	5
6.2 Loading Embeddings into Qdrant Vector Database	6
6.3 Launching Webservice	6
7 Answering Complex Queries	6
8 Predicting Missing Links	8
9 Downloading Pretrained Models	8
10 How to Deploy	8
11 Docker	8
12 Coverage Report	8
13 How to cite	10
14 dicee	12
14.1 Submodules	12
14.2 Attributes	169
14.3 Classes	170
14.4 Functions	171
14.5 Package Contents	172
Python Module Index	219

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

1 Dicee Manual

Version: dicee 0.2.0

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

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

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

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

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

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

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

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

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

² <https://github.com/Demirrr>

³ <https://pandas.pydata.org/>

⁴ <https://pytorch.org/>

⁵ <https://huggingface.co/>

⁶ <https://pandas.pydata.org/>

⁷ <https://pytorch.org/>

⁸ <https://pytorch.org/>

⁹ <https://www.pytorchlightning.ai/>

¹⁰ <https://huggingface.co/gradio>

2 Installation

2.1 Installation from Source

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

or

```
pip install dicee
```

3 Download Knowledge Graphs

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

To test the Installation

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

4 Knowledge Graph Embedding Models

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

For more, please refer to examples.

5 How to Train

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

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

where the data is in the following form

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

A KGE model can also be trained from the command line

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

dicee automatically detects available GPUs and trains a model with distributed data parallel technique. Under the hood, dicee uses lightning as a default trainer.

```
# Train a model by only using the GPU-0
CUDA_VISIBLE_DEVICES=0 dicee --dataset_dir "KGs/UMLS" --model Keci --eval_model
↪ "train_val_test"
# Train a model by only using GPU-1
CUDA_VISIBLE_DEVICES=1 dicee --dataset_dir "KGs/UMLS" --model Keci --eval_model
↪ "train_val_test"
NCCL_P2P_DISABLE=1 CUDA_VISIBLE_DEVICES=0,1 python dicee/scripts/run.py --trainer PL -
↪ --dataset_dir "KGs/UMLS" --model Keci --eval_model "train_val_test"
```

Under the hood, dicee executes run.py script and uses lightning as a default trainer

```
# Two equivalent executions
# (1)
dicee --dataset_dir "KGs/UMLS" --model Keci --eval_model "train_val_test"
# Evaluate Keci on Train set: Evaluate Keci on Train set
# {'H@1': 0.9518788343558282, 'H@3': 0.9988496932515337, 'H@10': 1.0, 'MRR': 0.
↪ 9753123402351737}
# Evaluate Keci on Validation set: Evaluate Keci on Validation set
# {'H@1': 0.6932515337423313, 'H@3': 0.9041411042944786, 'H@10': 0.9754601226993865,
↪ 'MRR': 0.8072362996241839}
# Evaluate Keci on Test set: Evaluate Keci on Test set
# {'H@1': 0.6951588502269289, 'H@3': 0.9039334341906202, 'H@10': 0.9750378214826021,
↪ 'MRR': 0.8064032293278861}

# (2)
CUDA_VISIBLE_DEVICES=0,1 python dicee/scripts/run.py --trainer PL --dataset_dir "KGs/
↪ UMLS" --model Keci --eval_model "train_val_test"
# Evaluate Keci on Train set: Evaluate Keci on Train set
# {'H@1': 0.9518788343558282, 'H@3': 0.9988496932515337, 'H@10': 1.0, 'MRR': 0.
↪ 9753123402351737}
# Evaluate Keci on Train set: Evaluate Keci on Train set
# Evaluate Keci on Validation set: Evaluate Keci on Validation set
# {'H@1': 0.6932515337423313, 'H@3': 0.9041411042944786, 'H@10': 0.9754601226993865,
↪ 'MRR': 0.8072362996241839}
# Evaluate Keci on Test set: Evaluate Keci on Test set
# {'H@1': 0.6951588502269289, 'H@3': 0.9039334341906202, 'H@10': 0.9750378214826021,
↪ 'MRR': 0.8064032293278861}
```

Similarly, models can be easily trained with torchrun

```

torchrun --standalone --nnodes=1 --nproc_per_node=gpu dicee/scripts/run.py --trainer_
↪torchDDP --dataset_dir "KGs/UMLS" --model Keci --eval_model "train_val_test"
# Evaluate Keci on Train set: Evaluate Keci on Train set: Evaluate Keci on Train set
# {'H@1': 0.9518788343558282, 'H@3': 0.9988496932515337, 'H@10': 1.0, 'MRR': 0.
↪9753123402351737}
# Evaluate Keci on Validation set: Evaluate Keci on Validation set
# {'H@1': 0.6932515337423313, 'H@3': 0.9041411042944786, 'H@10': 0.9754601226993865,
↪'MRR': 0.8072499937521418}
# Evaluate Keci on Test set: Evaluate Keci on Test set
{'H@1': 0.6951588502269289, 'H@3': 0.9039334341906202, 'H@10': 0.9750378214826021,
↪'MRR': 0.8064032293278861}

```

You can also train a model in multi-node multi-gpu setting.

```

torchrun --nnodes 2 --nproc_per_node=gpu --node_rank 0 --rdzv_id 455 --rdzv_backend_
↪c10d --rdzv_endpoint=nebula dicee/scripts/run.py --trainer torchDDP --dataset_dir_
↪KGs/UMLS
torchrun --nnodes 2 --nproc_per_node=gpu --node_rank 1 --rdzv_id 455 --rdzv_backend_
↪c10d --rdzv_endpoint=nebula dicee/scripts/run.py --trainer torchDDP --dataset_dir_
↪KGs/UMLS

```

Train a KGE model by providing the path of a single file and store all parameters under newly created directory called KeciFamilyRun.

```

dicee --path_single_kg "KGs/Family/family-benchmark_rich_background.owl" --model Keci
↪--path_to_store_single_run KeciFamilyRun --backend rdflib

```

where the data is in the following form

```

$ head -3 KGs/Family/train.txt
_:1 <http://www.w3.org/1999/02/22-rdf-syntax-ns#type> <http://www.w3.org/2002/07/owl
↪#Ontology> .
<http://www.benchmark.org/family#hasChild> <http://www.w3.org/1999/02/22-rdf-syntax-ns
↪#type> <http://www.w3.org/2002/07/owl#ObjectProperty> .
<http://www.benchmark.org/family#hasParent> <http://www.w3.org/1999/02/22-rdf-syntax-
↪ns#type> <http://www.w3.org/2002/07/owl#ObjectProperty> .

```

Apart from n-triples or standard link prediction dataset formats, we support [“owl”, “nt”, “turtle”, “rdf/xml”, “n3”]*. Moreover, a KGE model can be also trained by providing an endpoint of a triple store.

```

dicee --sparql_endpoint "http://localhost:3030/mutagenesis/" --model Keci

```

For more, please refer to examples.

6 Creating an Embedding Vector Database

6.1 Learning Embeddings

```

# Train an embedding model
dicee --dataset_dir KGs/Countries-S1 --path_to_store_single_run CountryEmbeddings --
↪model Keci --p 0 --q 1 --embedding_dim 32 --adaptive_swa

```

6.2 Loading Embeddings into Qdrant Vector Database

```
# Ensure that Qdrant available
# docker pull qdrant/qdrant && docker run -p 6333:6333 -p 6334:6334      -v $(pwd) /
→qdrant_storage:/qdrant/storage:z      qdrant/qdrant
diceeindex --path_model "CountryEmbeddings" --collection_name "dummy" --location
→"localhost"
```

6.3 Launching Webservice

```
diceeserve --path_model "CountryEmbeddings" --collection_name "dummy" --collection_
→location "localhost"
```

Retrieve and Search

Get embedding of germany

```
curl -X 'GET' 'http://0.0.0.0:8000/api/get?q=germany' -H 'accept: application/json'
```

Get most similar things to europe

```
curl -X 'GET' 'http://0.0.0.0:8000/api/search?q=europe' -H 'accept: application/json'
{"result": [{"hit": "europe", "score": 1.0},
 {"hit": "northern_europe", "score": 0.67126536},
 {"hit": "western_europe", "score": 0.6010134},
 {"hit": "puerto_rico", "score": 0.5051694},
 {"hit": "southern_europe", "score": 0.4829831}]}
```

7 Answering Complex Queries

```
# pip install dicee
# wget https://files.dice-research.org/datasets/dice-embeddings/KGs.zip --no-check-
→certificate & unzip KGs.zip
from dicee.executer import Execute
from dicee.config import Namespace
from dicee.knowledge_graph_embeddings import KGE
# (1) Train a KGE model
args = Namespace()
args.model = 'Keci'
args.p=0
args.q=1
args.optim = 'Adam'
args.scoring_technique = "AllvsAll"
args.path_single_kg = "KGs/Family/family-benchmark_rich_background.owl"
args.backend = "rdflib"
args.num_epochs = 200
args.batch_size = 1024
args.lr = 0.1
args.embedding_dim = 512
result = Execute(args).start()
# (2) Load the pre-trained model
```

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

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

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

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

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

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

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

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

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

For more, please refer to examples/multi_hop_query_answering.

8 Predicting Missing Links

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

9 Downloading Pretrained Models

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

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

10 How to Deploy

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

11 Docker

To build the Docker image:

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

To test the Docker image:

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

12 Coverage Report

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

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

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

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

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

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

13 How to cite

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

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

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

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

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

14 dicee

14.1 Submodules

dicee.__main__

dicee.abstracts

Classes

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

Module Contents

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

Abstract class for Trainer class for knowledge graph embedding models

Parameter

args
[str] ?

callbacks: list
?

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

A function to call callbacks before the training starts.

Parameter

args

kwargs

rtype

None

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

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

Parameter

args

kwargs

rtype

None

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

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

Parameter

args

kwargs

rtype

None

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

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

Parameter

args

kwargs

rtype

None

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

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

Parameter

args

kwargs

rtype

None

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

A static function to save a model into disk

Parameter

full_path : str

model:

rtype

None

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

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

Parameter

```
path_of_pretrained_model_dir  
[str] ?
```

```
construct_ensemble: boolean  
?
```

model_name: str apply_semantic_constraint : boolean

```
construct_ensemble = False
```

```
apply_semantic_constraint = False
```

configs

```
get_eval_report() → dict
```

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

Parameters

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

Return type

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

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

Parameters

triples

set_model_train_mode() → None
Setting the model into training mode

Parameter

set_model_eval_mode() → None
Setting the model into eval mode

Parameter

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

Parameter

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

Returns: Tuple

pytorch tensor of triple score

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

Parameter

items:
entities

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

Parameter

items:

relations

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

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

parameters ()

class dicee.abstracts.**InteractiveQueryDecomposition**

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

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

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

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

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

class dicee.abstracts.**AbstractCallback**

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

Abstract class for Callback class for knowledge graph embedding models

Parameter

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

Parameter

trainer:

model:

rtype

None

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

Call at the beginning of the training.

Parameter

trainer:

model:

rtype

None

on_fit_start (*trainer*, *model*)

Call at the beginning of the training.

Parameter

trainer:

model:

rtype

None

on_train_epoch_end(*trainer, model*)

Call at the end of each epoch during training.

Parameter

trainer:

model:

rtype

None

on_train_batch_end(**args, **kwargs*)

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

Parameter

trainer:

model:

rtype

None

on_fit_end(**args, **kwargs*)

Call at the end of the training.

Parameter

trainer:

model:

rtype

None

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

Bases: *AbstractCallback*

Abstract class for Callback class for knowledge graph embedding models

Parameter

num_epochs

path

sample_counter = 0

```

epoch_count = 0
alphas = None

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

```

Parameter

trainer:

model:

rtype

None

```

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

```

Parameter

trainer:

model:

rtype

None

```

store_ensemble(param_ensemble) → None

```

```

class dicee.abstracts.BaseInteractiveTrainKGE

```

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

```

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

```

```

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

```

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

```

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

```

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

```

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

```

Trains the Literal Embeddings model using literal data.

Parameters

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

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

dicee.analyse_experiments

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

Classes

Experiment

Functions

get_default_arguments()
analyse(args)

Module Contents

```
dicee.analyse_experiments.get_default_arguments()

class dicee.analyse_experiments.Experiment

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

```
full_storage_path = []
pq = []
train_mrr = []
train_h1 = []
train_h3 = []
train_h10 = []
val_mrr = []
val_h1 = []
val_h3 = []
val_h10 = []
test_mrr = []
test_h1 = []
test_h3 = []
test_h10 = []
runtime = []
normalization = []
scoring_technique = []
save_experiment(x)
to_df()

dicee.analyse_experiments.analyse(args)
```

dicee.callbacks

Classes

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

Functions

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

Module Contents

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

Bases: `dicee.abstracts.AbstractCallback`

Abstract class for Callback class for knowledge graph embedding models

Parameter

`path`

`on_fit_end(trainer, model) → None`

Store epoch loss

Parameter

trainer:

model:

`rtype`

None

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

Parameter

start_time

on_fit_start (*trainer, pl_module*)

Call at the beginning of the training.

Parameter

trainer:

model:

rtype

None

on_fit_end (*trainer, pl_module*)

Call at the end of the training.

Parameter

trainer:

model:

rtype

None

on_train_batch_end (**args, **kwargs*)

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

Parameter

trainer:

model:

rtype

None

on_train_epoch_end (**args, **kwargs*)

Call at the end of each epoch during training.

Parameter

trainer:

model:

rtype

None

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

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

Abstract class for Callback class for knowledge graph embedding models

Parameter

every_x_epoch

max_epochs

epoch_counter = 0

path

on_train_batch_end(*args, **kwargs)

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

Parameter

trainer:

model:

rtype

None

on_fit_start(trainer, pl_module)

Call at the beginning of the training.

Parameter

trainer:

model:

rtype

None

on_train_epoch_end(*args, **kwargs)

Call at the end of each epoch during training.

Parameter

trainer:

model:

rtype

None

on_fit_end(*args, **kwargs)

Call at the end of the training.

Parameter

trainer:

model:

rtype

None

on_epoch_end(model, trainer, **kwargs)

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

Bases: dicee.abstracts.AbstractCallback

Abstract class for Callback class for knowledge graph embedding models

Parameter

data_module

kg

num_of_epochs = 0

unlabelled_size

batch_size

create_random_data()

on_epoch_end(trainer, model)

dicee.callbacks.estimate_q(eps)

estimate rate of convergence q from sequence esp

dicee.callbacks.compute_convergence(seq, i)

class dicee.callbacks.ASWA(num_epochs, path)

Bases: dicee.abstracts.AbstractCallback

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

path

num_epochs

initial_eval_setting = None

epoch_count = 0

alphas = []

val_aswa = -1

on_fit_end(trainer, model)

Call at the end of the training.

Parameter

trainer:

model:

rtype

None

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

Perform Hard Update, software or rejection

Parameters

- running_model_state_dict
- ensemble_state_dict
- val_running_model
- mrr_updated_ensemble_model

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

Call at the end of each epoch during training.

Parameter

trainer:

model:

rtype

None

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

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

Abstract class for Callback class for knowledge graph embedding models

Parameter

path

reports = []

epoch_ratio = None

epoch_counter = 0

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

Call at the beginning of the training.

Parameter

trainer:

model:

rtype

None

on_fit_end(*trainer, model*)

Call at the end of the training.

Parameter

trainer:

model:

rtype

None

on_train_epoch_end(*trainer, model*)

Call at the end of each epoch during training.

Parameter

trainer:

model:

rtype

None

on_train_batch_end(*args, **kwargs)

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

Parameter

trainer:

model:

rtype

None

class dicee.callbacks.Krone

Bases: *dicee.abstracts.AbstractCallback*

Abstract class for Callback class for knowledge graph embedding models

Parameter

f = None

static batch_kronecker_product(*a, b*)

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

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

Get kronecker embeddings

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

Call at the beginning of the training.

Parameter

trainer:

model:

rtype

None

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

Bases: *dicee.abstracts.AbstractCallback*

A callback for a three-Level Perturbation

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

Parameter Perturbation:

Output Perturbation:

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

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

Called when the train batch begins.

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

Bases: *dicee.abstracts.AbstractCallback*

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

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

```
experiment_dir
```

```
max_epochs
```

```
epoch_counter = 0
```

```
save_model_every_n_epoch = True
```

```
reports
```

```

n_epochs_eval_model = 'val_test'

default_eval_model = None

eval_epochs

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

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

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

Callback for managing learning rate scheduling and model snapshots.

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

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

total_epochs

experiment_dir

snapshot_dir

batches_per_epoch = None

total_steps = None

cycle_length = None

warmup_steps = None

lr_lambda = None

scheduler = None

step_count = 0

snapshot_loss

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

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

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

```

Parameter

trainer:

model:

rtype

None

```

class dicee.callbacks.SWA(swa_start_epoch, swa_c_epochs: int = 1, lr_init: float = 0.1,
                           swa_lr: float = 0.05, max_epochs: int = None)
Bases: dicee.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

moving_average(swa_model, model, alpha)
    Update SWA model with moving average of current model.

on_fit_start(trainer, model)
    Initialize SWA model with same architecture as main model.

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

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

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

```

dicee.config

Classes

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

Module Contents

```

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

Simple object for storing attributes.

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

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

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

```

```

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

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

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

sparql_endpoint = None
    An endpoint of a triple store.

model: str = 'Keci'
    KGE model

optim: str = 'Adam'
    Optimizer

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

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

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

lr: float = 0.1
    Learning rate

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

gpus = None
    Number GPUs to be used during training

callbacks
    10}

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

        Type
            {"last_percent_to_consider"}

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

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

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

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

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

```

```

weight_decay: float = 0.0
    Weight decay for all trainable params

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

init_param: str = None
    xavier_normal or None

gradient_accumulation_steps: int = 0
    Not tested e

num_folds_for_cv: int = 0
    Number of folds for CV

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

Type
    Evaluate trained model choices

save_model_at_every_epoch: int = None
    Not tested

label_smoothing_rate: float = 0.0

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

random_seed: int = 0
    Random Seed

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

read_only_few: int = None
    Read only first few triples

pykeen_model_kwargs
    Additional keyword arguments for pykeen models

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

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

p: int = 0
    P parameter of Clifford Embeddings

q: int = 1
    Q parameter of Clifford Embeddings

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

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

```

```

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

byte_pair_encoding: bool = False
    Byte pair encoding

    Type
        WIP

adaptive_swa: bool = False
    Adaptive stochastic weight averaging

swa: bool = False
    Stochastic weight averaging

block_size: int = None
    block size of LLM

continual_learning = None
    Path of a pretrained model size of LLM

auto_batch_finding = False
    A flag for using auto batch finding

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

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

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

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

adaptive_lr
    "cca"}'

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

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

__iter__()

dicee.dataset_classes

```

Classes

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

Functions

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

Module Contents

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

Reload the files from disk to construct the Pytorch dataset

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

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

Bases: torch.utils.data.Dataset

An abstract class representing a Dataset.

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

Note

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

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

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

Bases: `torch.utils.data.Dataset`

An abstract class representing a `Dataset`.

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

Note

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

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

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

Bases: torch.utils.data.Dataset

Dataset for the 1vsALL training strategy

Parameters

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

Return type

torch.utils.data.Dataset

train_data

block_size = 8

num_of_data_points

collate_fn = None

__len__()

__getitem__(idx)

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

Bases: torch.utils.data.Dataset

Dataset for the 1vsALL training strategy

Parameters

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

Return type

torch.utils.data.Dataset

train_data

target_dim

collate_fn = None

__len__()

__getitem__(idx)

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

Bases: torch.utils.data.Dataset

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

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

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

Note

TODO

train_set_idx

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

entity_idxs

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

relation_idxs

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

self : torch.utils.data.Dataset

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

```
train_data = None
```

```
train_target = None
```

```
label_smoothing_rate
```

```
collate_fn = None
```

```
__len__()
```

```
__getitem__(idx)
```

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

Bases: torch.utils.data.Dataset

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

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

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

Note

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

```

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

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

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

self : torch.utils.data.Dataset

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

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

class dicee.dataset_classes.OnevsSample(train_set: numpy.ndarray, num_entities, num_relations, neg_sample_ratio: int = None, label_smoothing_rate: float = 0.0)
Bases: torch.utils.data.Dataset

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

Parameters

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

train_data

The input data converted into a PyTorch tensor.

Type
torch.Tensor

```

num_entities
    Number of entities in the dataset.

    Type
        int

num_relations
    Number of relations in the dataset.

    Type
        int

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

    Type
        int

label_smoothing_rate
    The smoothing factor applied to the labels.

    Type
        torch.Tensor

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

    Type
        function, optional

train_data

num_entities

num_relations

neg_sample_ratio = None

label_smoothing_rate

collate_fn = None

__len__()
    Returns the number of samples in the dataset.

__getitem__(idx)
    Retrieves a single data sample from the dataset at the given index.

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

Returns
    A tuple consisting of:
    

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

```

Return type

tuple

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

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

Bases: torch.utils.data.Dataset

KvsSample a Dataset:**D:= {(x,y)_i}_i ^N, where**

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

orall y_i =1 s.t. (h r E_i) in KG**At each mini-batch construction, we subsample(y), hence n****|new_y| << |E| new_y contains all 1's if sum(y)< neg_sample ratio new_y contains****train_set_idx**

Indexed triples for the training.

entity_idxs

mapping.

relation_idxs

mapping.

form

?

store

?

label_smoothing_rate

?

torch.utils.data.Dataset

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

```
class dicee.dataset_classes.NegSampleDataset (train_set: numpy.ndarray, num_entities: int,  

    num_relations: int, neg_sample_ratio: int = 1)
```

Bases: torch.utils.data.Dataset

An abstract class representing a Dataset.

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

Note

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

```
neg_sample_ratio
train_set
length
num_entities
num_relations
__len__()
__getitem__(idx)

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

Triple Dataset
D:= {(x)_i}_i ^N, where
    . x:(h,r, t) in KG is a unique h in E and a relation r in R and . collect_fn => Generates
        negative triples
    collect_fn:
        orall (h,r,t) in G obtain, create negative triples{(h,r,x),(r,t),(h,m,t)}
        y:labels are represented in torch.float16

train_set_idx
    Indexed triples for the training.

entity_idxs
    mapping.

relation_idxs
    mapping.

form
?
store
?

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

```

label_smoothing_rate
neg_sample_ratio
train_set
length
num_entities
num_relations

__len__()
__getitem__(idx)
collate_fn(batch: List[torch.Tensor])

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

```

Create a Dataset for cross validation

Parameters

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

Return type

?

```

train_set_idx
num_entities
num_relations
neg_sample_ratio
batch_size
num_workers

train_dataloader() → torch.utils.data.DataLoader

```

An iterable or collection of iterables specifying training samples.

For more information about multiple dataloaders, see this section.

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

For data processing use the following pattern:

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

However, the above are only necessary for distributed processing.

⚠ Warning

do not assign state in `prepare_data`

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

ℹ Note

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

`setup(*args, **kwargs)`

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

Parameters

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

Example:

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

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

        # don't do this
        self.something = else

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

`transfer_batch_to_device(*args, **kwargs)`

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

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

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

- tuple

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

Note

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

Parameters

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

Returns

A reference to the data on the new device.

Example:

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

See also

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

`prepare_data(*args, **kwargs)`

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

Warning

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

Example:

```

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

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

```

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

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

Example:

```

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

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

```

This is called before requesting the dataloaders:

```

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

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

```

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

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

`train_file_path`

Path to the training data file.

Type

str

```

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

    Type
        str

normalization_params
    Parameters used for normalization.

    Type
        dict

sampling_ratio
    Fraction of the training set to use for ablations.

    Type
        float

entity_to_idx
    Mapping of entities to their indices.

    Type
        dict

num_entities
    Total number of entities.

    Type
        int

data_property_to_idx
    Mapping of data properties to their indices.

    Type
        dict

num_data_properties
    Total number of data properties.

    Type
        int

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

    Type
        str

train_file_path
loader_backend = 'pandas'
normalization_type = 'z-norm'
normalization_params
sampling_ratio = None
entity_to_idx = None
num_entities

```

```

__getitem__(index)

__len__()

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

Returns
    DataFrame containing the loaded and validated data.

Return type
    pd.DataFrame

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

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

Returns
    Denormalized predictions.

Return type
    np.ndarray

```

dicee.eval_static_funcs

Functions

<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,</code>	triples[,
<code>er_vocab, ...])</code>	
<code>evaluate_literal_prediction(kge_model[, ...])</code>	Evaluates the trained literal prediction model on a test file.
<code>evaluate_ensemble_link_prediction_performa</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) → Dict
```

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

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

Parameters

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

Returns

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

dicee.evaluator

Classes

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

Module Contents

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

Evaluator class to evaluate KGE models in various downstream tasks

Arguments

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

args

report

during_training = False

vocab_preparation(dataset) → None

A function to wait future objects for the attributes of executor

Return type

None

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

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

```

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

```

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

```

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

```

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

```

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

```

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

```

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

Parameters

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

```
evaluate_lp(model, triple_idx, info: str)
```

```
dummy_eval(trained_model, form_of_labelling: str)
```

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

dicee.executer

Classes

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

Module Contents

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

A class for Training, Retraining and Evaluation a model.

- (1) Loading & Preprocessing & Serializing input data.
- (2) Training & Validation & Testing
- (3) Storing all necessary info

```
args
```

```

is_continual_training = False
trainer = None
trained_model = None
knowledge_graph = None
report
evaluator = None
start_time = None
setup_executor() → None
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

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

Module Contents

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

__str__()

to(device: str) → None

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

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

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

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

predict_missing_head_entity(relation: List[str] | str, tail_entity: List[str] | str, within=None,
                            batch_size=2, topk=1, return_indices=False) → Tuple
Given a relation and a tail entity, return top k ranked head entity.

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

Parameter

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

Returns: Tuple

Highest K scores and entities

```
predict_missing_relations(head_entity: List[str] | str, tail_entity: List[str] | str, within=None,
                           batch_size=2, topk=1, return_indices=False) → Tuple
Given a head entity and a tail entity, return top k ranked relations.

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

Parameter

head_entity: List[str]

String representation of selected entities.

tail_entity: List[str]

String representation of selected entities.

k: int

Highest ranked k entities.

Returns: Tuple

Highest K scores and entities

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

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

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

Parameter

head_entity: List[str]

String representation of selected entities.

tail_entity: List[str]

String representation of selected entities.

Returns: Tuple

scores

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

Parameters

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

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

Predict missing item in a given triple.

Returns

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

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

Parameter

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

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

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

logits: bool
If logits is True, unnormalized score returned

Returns: Tuple

pytorch tensor of triple score

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

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

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

Find an answer set for EPFO queries including negation and disjunction

Parameter

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

query: Union[str, Tuple[str, Tuple[str, Tuple[str, str]]]] The query itself, either a string or a nested tuple.

queries: List of Tuple[Union[str, Tuple[str, str]], ...]

tnorm: str The t-norm operator.

neg_norm: str The negation norm.

lambda_: float lambda parameter for sugeno and yager negation norms

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

returns

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

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

Find missing triples

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

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

Return (e,r,x)

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

confidence: float

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

topk: int

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

at_most: int

Stop after finding at_most missing triples

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

otin G

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

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

Predicts literal values for given entities and attributes.

Parameters

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

Returns

Predictions for the given entities and attributes.

Return type

numpy ndarray

dicee.models

Submodules

dicee.models.adopt

Classes

ADOPT

Base class for all optimizers.

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`

Base class for all optimizers.

⚠ Warning

Parameters need to be specified as collections that have a deterministic ordering that is consistent between runs. Examples of objects that don't satisfy those properties are sets and iterators over values of dictionaries.

Parameters

- **params** (`iterable`) – an iterable of `torch.Tensor`s or `dict`s. Specifies what Tensors should be optimized.
- **defaults** – (`dict`): a dict containing default values of optimization options (used when a parameter group doesn't specify them).

`clip_lambda`

`__setstate__(state)`

`step(closure=None)`

Perform a single optimization step.

Parameters

`closure` (`Callable, optional`) – A closure that reevaluates the model and returns the loss.

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

Functional API that performs ADOPT algorithm computation.

dicee.models.base_model

Classes

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

Module Contents

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

Bases: `lightning.LightningModule`

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

Note

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

Variables

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

`training_step_outputs` = []

`mem_of_model()` → Dict

Size of model in MB and number of params

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

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

Parameters

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

Returns

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

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

Example:

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

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

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

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

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

Note

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

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

Parameters

- `yhat_batch`

- `y_batch`

`on_train_epoch_end(*args, **kwargs)`

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

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

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

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

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

`test_epoch_end(outputs: List[Any])`

`test_dataloader() → None`

An iterable or collection of iterables specifying test samples.

For more information about multiple dataloaders, see this section.

For data processing use the following pattern:

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

However, the above are only necessary for distributed processing.

⚠ Warning

do not assign state in `prepare_data`

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

ℹ Note

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

Note

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

`val_dataloader() → None`

An iterable or collection of iterables specifying validation samples.

For more information about multiple dataloaders, see this section.

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

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

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

Note

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

Note

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

`predict_dataloader() → None`

An iterable or collection of iterables specifying prediction samples.

For more information about multiple dataloaders, see this section.

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

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

Note

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

Returns

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

`train_dataloader() → None`

An iterable or collection of iterables specifying training samples.

For more information about multiple dataloaders, see this section.

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

For data processing use the following pattern:

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

However, the above are only necessary for distributed processing.

Warning

do not assign state in `prepare_data`

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

Note

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

`configure_optimizers(parameters=None)`

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

Returns

Any of these 6 options.

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

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

```

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

```

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

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

Note

Some things to know:

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

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

Bases: `BaseKGELightning`

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

Note

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

Variables

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

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

```

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

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

Parameters
-----
init_params_with_sanity_checking()

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


- x
- y_idx
- ordered_bpe_entities

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

Parameters
-----
x
forward_k_vs_all(*args, **kwargs)
forward_k_vs_sample(*args, **kwargs)

```

```

get_triple_representation(idx_hrt)
get_head_relation_representation(indexed_triple)
get_sentence_representation(x: torch.LongTensor)

Parameters

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

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

```

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

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

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

Bases: torch.nn.Module

Base class for all neural network modules.

Your models should also subclass this class.

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

```

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

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

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

```

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

Note

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

Variables

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

```

args = None

__call__(x)

static forward(x)

```

dicee.models.clifford

Classes

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

Module Contents

```

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

```

Base class for all neural network modules.

Your models should also subclass this class.

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

```

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

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

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

```

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

Note

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

Variables

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

```

name = 'Keci'

```

```

p
q
r

requires_grad_for_interactions = True

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

    Yet, this computation would be quite inefficient. Instead, we compute interactions along all p, e.g., e1e1,
    e1e2, e1e3,
    e2e1, e2e2, e2e3, e3e1, e3e2, e3e3

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

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

    Yet, this computation would be quite inefficient. Instead, we compute interactions along all p, e.g., e1e1,
    e1e2, e1e3,
    e2e1, e2e2, e2e3, e3e1, e3e2, e3e3

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

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

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

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

```

```

h = h_0 + sum_{i=1}^p h_i e_i + sum_{j=p+1}^{p+q} h_j e_j r = r_0 + sum_{i=1}^p r_i e_i +
sum_{j=p+1}^{p+q} r_j e_j
ei ^2 = +1 for i <= p ej ^2 = -1 for p < j <= p+q ei ej = -eje1 for i

```

eq j

```

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

```

construct_cl_multivector (x: `torch.FloatTensor`, r: `int`, p: `int`, q: `int`)
 \rightarrow tuple[`torch.FloatTensor`, `torch.FloatTensor`, `torch.FloatTensor`]

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

Parameter

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

returns

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

forward_k_vs_with_explicit (x: `torch.Tensor`)

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

forward_k_vs_all (x: `torch.Tensor`) \rightarrow `torch.FloatTensor`

Kvsall training

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

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

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

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

Parameter

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

returns

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

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

Parameter

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

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

rtype

torch.FloatTensor with (n, k) shape

score (*h, r, t*)

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

Parameter

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

rtype

torch.FloatTensor with (n) shape

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

Bases: *Keci*

Without learning dimension scaling

name = 'CKeci'

requires_grad_for_interactions = False

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

Bases: *dicee.models.base_model.BaseKGE*

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

Note

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

Variables

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

```
name = 'DeCaL'

entity_embeddings

relation_embeddings

p

q

r

re

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

Parameter

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

`rtype`

`torch.FloatTensor with (n) shape`

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

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

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

`compute_sigmas_single (list_h_emb, list_r_emb, list_t_emb)`

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

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

and return:

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

compute_sigmas_multivect (*list_h_emb*, *list_r_emb*)

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

For same bases vectors interaction we have

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

For different base vector interactions, we have

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

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

Kvsall training

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

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

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

Multiplying a base vector with its scalar coefficient

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

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

Parameter

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

returns

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

compute_sigma_pp (*hp, rp*)

Compute .. math:

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

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

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

```

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

```

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

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

e2e1, e2e2, e2e3, e3e1, e3e2, e3e3

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

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

Compute

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

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

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

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

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

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

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

e2e1, e2e2, e2e3, e3e1, e3e2, e3e3

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

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

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

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

Compute

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

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

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

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

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

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

Compute

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

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

```

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

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


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


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

```

dicee.models.complex

Classes

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

Module Contents

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

Bases: `dicee.models.base_model.BaseKGE`

Convolutional ComplEx Knowledge Graph Embeddings

`name` = 'ConEx'

`conv2d`

`fc_num_input`

`fc1`

`norm_fc1`

`bn_conv2d`

`feature_map_dropout`

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

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

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

```

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

Parameters
    x

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

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

    conv2d
    fc_num_input
    fc1
    norm_fc1
    bn_conv2d
    feature_map_dropout

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

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

Parameters
    x

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

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

    Your models should also subclass this class.

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

```

```

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

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

```

(continues on next page)

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

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

Note

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

Variables

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

```
name = 'Complex'

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

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

Parameters

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

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

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

dicee.models.dualE

Classes

`DualE`

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

Module Contents

`class dicee.models.dualE.DualE(args)`

Bases: `dicee.models.base_model.BaseKGE`

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

`name = 'DualE'`

```
entity_embeddings
relation_embeddings
num_ent = None
kvsall_score(e_1_h, e_2_h, e_3_h, e_4_h, e_5_h, e_6_h, e_7_h, e_8_h, e_1_t, e_2_t, e_3_t, e_4_t,
    e_5_t, e_6_t, e_7_t, e_8_t, r_1, r_2, r_3, r_4, r_5, r_6, r_7, r_8) → torch.tensor
    KvsAll scoring function
```

Input

x: torch.LongTensor with (n,) shape

Output

torch.FloatTensor with (n) shape

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

Negative Sampling forward pass:

Input

x: torch.LongTensor with (n,) shape

Output

torch.FloatTensor with (n) shape

```
forward_k_vs_all(x)
```

KvsAll forward pass

Input

x: torch.LongTensor with (n,) shape

Output

torch.FloatTensor with (n) shape

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

Transpose function

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

dicee.models.ensemble

Classes

```
EnsembleKGE
```

Module Contents

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

    name
    train_mode = True
    named_children()
    property example_input_array
    parameters()
    modules()
    __iter__()
    __len__()
    eval()
    to(device)
    mem_of_model()
    __call__(x_batch)
    step()
    get_embeddings()
    __str__()

dicee.models.function_space
```

Classes

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

Module Contents

```
class dicee.models.function_space.FMult(args)
Bases: dicee.models.base_model.BaseKGE
Learning Knowledge Neural Graphs
name = 'FMult'
entity_embeddings
```

```

relation_embeddings

k

num_sample = 50

gamma

roots

weights

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

chain_func (weights, x: torch.FloatTensor)

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

Parameters

x

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

Learning Knowledge Neural Graphs

name = 'GFMult'

entity_embeddings

relation_embeddings

k

num_sample = 250

roots

weights

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

chain_func (weights, x: torch.FloatTensor)

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

Parameters

x

class dicee.models.function_space.FMult2 (args)
Bases: dicee.models.base_model.BaseKGE

Learning Knowledge Neural Graphs

name = 'FMult2'

n_layers = 3

k

n = 50

```

```

score_func = 'compositional'

discrete_points

entity_embeddings

relation_embeddings

build_func (Vec)

build_chain_funcs (list_Vec)

compute_func (W, b, x) → torch.FloatTensor

function (list_W, list_b)

trapezoid (list_W, list_b)

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

```

Parameters

x

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

Bases: *dicee.models.base_model.BaseKGE*

Embedding with trigonometric functions. We represent all entities and relations in the complex number space as: $f(x) = \sum_{k=0}^{\infty} \sum_{k=d-1}^d w_k e^{ikx}$. 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: $f(x) = \sum_{i=0}^{\infty} \sum_{d=1}^D a_{i,d} x^{i \% d}$ 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, coeffh, coeffr, coefft)
    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 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

<i>LiteralEmbeddings</i>	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

<i>octonion_mul</i> (* , O_1, O_2)
<i>octonion_mul_norm</i> (* , O_1, O_2)

Module Contents

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

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

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

Note

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

Variables

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

```
name = 'OMult'

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

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

k_vs_all_score(bpe_head_ent_emb, bpe_rel_ent_emb, E)
```

`forward_k_vs_all(x)`

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

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

Bases: *dicee.models.base_model.BaseKGE*

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

Note

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

Variables

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

```
name = 'Conv0'

conv2d

fc_num_input

fc1

bn_conv2d

norm_fc1

feature_map_dropout

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

residual_convolution(O_1, O_2)

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

Parameters

`x`

`forward_k_vs_all(x: torch.Tensor)`

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

```

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

        conv2d
        fc_num_input
        fc1
        bn_conv2d
        norm_fc1
        feature_map_dropout
        static octonion_normalizer(emb_rel_e0, emb_rel_e1, emb_rel_e2, emb_rel_e3, emb_rel_e4,
            emb_rel_e5, emb_rel_e6, emb_rel_e7)
        residual_convolution(O_1, O_2)
        forward_triples(x: torch.Tensor) → torch.Tensor

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

dicee.models.pykeen_models

```

Classes

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

Module Contents

```

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

```

```

loss_history = []

args

entity_embeddings = None

relation_embeddings = None

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

else:
    t = self.entity_embeddings.weight

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

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

abstract forward_k_vs_sample(x: torch.LongTensor, target_entity_idx)

```

dicee.models.quaternion

Classes

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

Functions

<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

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

dicee.models.static_funcs

Functions

quaternion_mul (→ Tuple[<i>torch.Tensor</i> , <i>torch.Tensor</i> , ...])	Perform quaternion multiplication
---	-----------------------------------

Module Contents

dicee.models.static_funcs.quaternion_mul (*Q_1, Q_2)	→ Tuple[<i>torch.Tensor</i> , <i>torch.Tensor</i> , <i>torch.Tensor</i> , <i>torch.Tensor</i>]
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) hugging-face/transformers PyTorch implementation: https://github.com/huggingface/transformers/blob/main/src/transformers/models/gpt2/modeling_gpt2.py

Classes

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

Module Contents

```
class dicee.models.transformers.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.**CausalSelfAttention** (*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
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

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>	Base class for all optimizers.
<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>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>BaseKGE</i>	Base class for all neural network modules.
<i>ConEx</i>	Convolutional ComplEx Knowledge Graph Embeddings
<i>AConEx</i>	Additive Convolutional ComplEx Knowledge Graph Embeddings
<i>ComplEx</i>	Base class for all neural network modules.
<i>BaseKGE</i>	Base class for all neural network modules.
<i>IdentityClass</i>	Base class for all neural network modules.
<i>QMult</i>	Base class for all neural network modules.
<i>ConvQ</i>	Convolutional Quaternion Knowledge Graph Embeddings
<i>AConvQ</i>	Additive Convolutional Quaternion Knowledge Graph Embeddings
<i>BaseKGE</i>	Base class for all neural network modules.
<i>IdentityClass</i>	Base class for all neural network modules.
<i>OMult</i>	Base class for all neural network modules.
<i>Convo</i>	Base class for all neural network modules.
<i>AConvO</i>	Additive Convolutional Octonion Knowledge Graph Embeddings
<i>Keci</i>	Base class for all neural network modules.
<i>CKeci</i>	Without learning dimension scaling
<i>DeCaL</i>	Base class for all neural network modules.
<i>BaseKGE</i>	Base class for all neural network modules.
<i>PykeenKGE</i>	A class for using knowledge graph embedding models implemented in Pykeen
<i>BaseKGE</i>	Base class for all neural network modules.
<i>FMult</i>	Learning Knowledge Neural Graphs
<i>GFMult</i>	Learning Knowledge Neural Graphs
<i>FMult2</i>	Learning Knowledge Neural Graphs

continues on next page

Table 1 – continued from previous page

<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
Base class for all optimizers.

```

⚠ Warning

Parameters need to be specified as collections that have a deterministic ordering that is consistent between runs. Examples of objects that don't satisfy those properties are sets and iterators over values of dictionaries.

Parameters

- **params** (*iterable*) – an iterable of *torch.Tensor*s or *dict*s. Specifies what Tensors should be optimized.
- **defaults** – (*dict*): a *dict* containing default values of optimization options (used when a parameter group doesn't specify them).

clip_lambda

__setstate__ (*state*)

step (*closure=None*)

Perform a single optimization step.

Parameters

`closure (Callable, optional)` – A closure that reevaluates the model and returns the loss.

`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 = ...
        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.
```

(continues on next page)

```

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

```

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

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

Note

Some things to know:

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

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

Bases: `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

```

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```

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

```

```

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

Parameters
x (B x 2 x T)

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

Parameters
-----
init_params_with_sanity_checking()

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

Parameters
• x
• y_idx
• ordered_bpe_entities

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

Parameters
x
forward_k_vs_all(*args, **kwargs)
forward_k_vs_sample(*args, **kwargs)
get_triple_representation(idx_hrt)
get_head_relation_representation(indexed_triple)

```

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

Parameters

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

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

Parameters

x (B x 2 x T)

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

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

Bases: torch.nn.Module

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

Note

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

Variables

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

```
args = None
```

```
__call__(x)
```

```
static forward(x)

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

Bases: *BaseKGELightning*

Base class for all neural network modules.

Your models should also subclass this class.

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

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

class Model(nn.Module):
    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.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.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)

```

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

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

Note

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

Variables

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

`args`

```
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

\mathbf{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.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.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):

```

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```
x = F.relu(self.conv1(x))
return F.relu(self.conv2(x))
```

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

Note

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

Variables

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

```
name = 'QMult'

explicit = True

quaternion_multiplication_followed_by_inner_product(h, r, t)
```

Parameters

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

Returns

Triple scores.

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

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

Absolute value of a quaternion

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

L2 norm of quaternion vector:

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

Parameters

`x` – The vector.

Returns

The normalized vector.

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

`k_vs_all_score (bpe_head_ent_emb, bpe_rel_ent_emb, E)`

Parameters

- `bpe_head_ent_emb`

- `bpe_rel_ent_emb`
- `E`

`forward_k_vs_all(x)`

Parameters

`x`

`forward_k_vs_sample(x, target_entity_idx)`

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

```

class dicee.models.ConvQ(args)
    Bases: dicee.models.base_model.BaseKGE
    Convolutional Quaternion Knowledge Graph Embeddings
    name = 'ConvQ'
    entity_embeddings
    relation_embeddings
    conv2d
    fc_num_input
    fc1
    bn_conv1
    bn_conv2
    feature_map_dropout
    residual_convolution(Q_1, Q_2)
    forward_triples(indexed_triple: torch.Tensor) → torch.Tensor

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

class dicee.models.AConvQ(args)
    Bases: dicee.models.base_model.BaseKGE
    Additive Convolutional Quaternion Knowledge Graph Embeddings
    name = 'AConvQ'
    entity_embeddings
    relation_embeddings
    conv2d

```

```

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

```

Parameters

`x`

`forward_k_vs_all(x: torch.Tensor)`

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

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

Bases: `BaseKGELightning`

Base class for all neural network modules.

Your models should also subclass this class.

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

```

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

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

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

```

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

Note

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

Variables

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

```

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

```

Parameters

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

```

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.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.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)

```

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

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

Note

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

Variables

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

`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.,
 $[score(h,r,x)|x \in Entities] \Rightarrow [0.0, 0.1, \dots, 0.8]$, shape $\Rightarrow (1, |Entities|)$ Given a batch of head entities and relations \Rightarrow shape (size of batch, $|Entities|$)

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

Bases: `dicee.models.base_model.BaseKGE`

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

Note

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

Variables

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

```
name = 'ConvO'

conv2d

fc_num_input

fc1

bn_conv2d

norm_fc1

feature_map_dropout

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

residual_convolution(O_1, O_2)

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

Parameters

`x`

`forward_k_vs_all(x: torch.Tensor)`

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

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

Bases: `dicee.models.base_model.BaseKGE`

Additive Convolutional Octonion Knowledge Graph Embeddings

```
name = 'AConvO'
```

```
conv2d
```

```
fc_num_input
```

```
fc1
```

```
bn_conv2d
```

```
norm_fc1
```

```
feature_map_dropout
```

```

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

residual_convolution(O_1, O_2)

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

Parameters
x

forward_k_vs_all(x: torch.Tensor)

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

class dicee.models.Keci(args)
Bases: dicee.models.base\_model.BaseKGE

Base class for all neural network modules.

Your models should also subclass this class.

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

```

```

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

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

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

```

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

Note

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

Variables

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

```

name = 'Keci'

p
q

```

```

r

requires_grad_for_interactions = True

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

    Yet, this computation would be quite inefficient. Instead, we compute interactions along all p, e.g., e1e1,
    e1e2, e1e3,
    e2e1, e2e2, e2e3, e3e1, e3e2, e3e3

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

compute_sigma_qq(hq, rq)
    Compute sigma_{qq} = sum_{j=1}^{p+q-1} sum_{k=j+1}^{p+q} (h_j r_k - h_k r_j) e_j e_k sigma_{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 = -ej ei for i
    eq j

```

$h \ r = \sigma_0 + \sigma_p + \sigma_q + \sigma_{pp} + \sigma_{q} + \sigma_{pq}$ where
(1) $\sigma_0 = h_0 r_0 + \sum_{i=1}^p (h_0 r_i) e_i - \sum_{j=p+1}^q (h_j r_j) e_j$
(2) $\sigma_p = \sum_{i=1}^p (h_0 r_i + h_i r_0) e_i$
(3) $\sigma_q = \sum_{j=p+1}^q (h_0 r_j + h_j r_0) e_j$
(4) $\sigma_{pp} = \sum_{i=1}^p \sum_{k=i+1}^q (h_i r_k - h_k r_i) e_i e_k$
(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) $\sigma_{pq} = \sum_{i=1}^p \sum_{j=p+1}^q (h_i r_j - h_j r_i) e_i e_j$

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

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

Parameter

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

returns

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

forward_k_vs_with_explicit (*x*: torch.Tensor)

k_vs_all_score (*bpe_head_ent_emb*, *bpe_rel_ent_emb*, *E*)

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

Kvsall training

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

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

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

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

Parameter

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

returns

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

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

Parameter

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

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

rtype

torch.FloatTensor with (n, k) shape

score (h, r, t)

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

Parameter

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

rtype

torch.FloatTensor with (n) shape

class dicee.models.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 submodules as regular attributes:

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

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

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

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

Note

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

Variables

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

```
name = 'DeCaL'

entity_embeddings
relation_embeddings

p
q
r
re

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

Parameter

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

rtype

`torch.FloatTensor` with `(n)` shape

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

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

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

`compute_sigmas_single(list_h_emb, list_r_emb, list_t_emb)`

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

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

and return:

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

`compute_sigmas_multivect(list_h_emb, list_r_emb)`

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

For same bases vectors interaction we have

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

For different base vector interactions, we have

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

forward_k_vs_all (*x*: *torch.FloatTensor*) → *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 : *torch.FloatTensor* with (n, |E|) shape

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

Multiplying a base vector with its scalar coefficient

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

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

Parameter

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

returns

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

compute_sigma_pp (*hp, rp*)

Compute .. math:

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

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

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

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

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

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

e2e1, e2e2, e2e3, e3e1, e3e2, e3e3

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

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

Compute

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

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

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

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

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

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

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

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

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

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

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

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

Compute

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

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

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

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

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

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

Compute

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

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

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

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

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

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

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

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

```

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

```

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

Bases: *BaseKGELightning*

Base class for all neural network modules.

Your models should also subclass this class.

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

```

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

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

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

```

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

Note

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

Variables

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

```

args
embedding_dim = None
num_entities = None
num_relations = None
num_tokens = None
learning_rate = None
apply_unit_norm = None
input_dropout_rate = None
hidden_dropout_rate = None

```

```

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

Parameters
x (B x 2 x T)

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

Parameters
-----
init_params_with_sanity_checking()

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

Parameters
• x
• y_idx
• ordered_bpe_entities

```

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

Parameters

x

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

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

```
get_triple_representation (idx_hrt)
```

```
get_head_relation_representation (indexed_triple)
```

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

Parameters

- (b (x shape)

- 3

- t)

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

→ Tuple[torch.FloatTensor, torch.FloatTensor]

Parameters

x (B x 2 x T)

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

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

Bases: dicee.models.base_model.BaseKGE

A class for using knowledge graph embedding models implemented in Pykeen

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

model_kwargs

name

model

loss_history = []

args

entity_embeddings = None

relation_embeddings = None

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

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

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

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

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

```

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

else:
    t = self.entity_embeddings.weight

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

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

abstract forward_k_vs_sample (x: torch.LongTensor, target_entity_idx)

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

Base class for all neural network modules.

Your models should also subclass this class.

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

```

```

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

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

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

```

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

Note

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

Variables

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

```

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

```

Parameters

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

```

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

    Parameters
    -----
    init_params_with_sanity_checking()

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

    Parameters
    • x
    • y_idx
    • ordered_bpe_entities

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

    Parameters
    x

    forward_k_vs_all(*args, **kwargs)

    forward_k_vs_sample(*args, **kwargs)

    get_triple_representation(idx_hrt)
    get_head_relation_representation(indexed_triple)
    get_sentence_representation(x: torch.LongTensor)

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

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

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

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

Learning Knowledge Neural Graphs

name = 'FMult'

entity_embeddings

relation_embeddings

k

```

```

num_sample = 50
gamma
roots
weights

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

Parameters
x

class dicee.models.GFMult (args)
Bases: dicee.models.base_model.BaseKGE
Learning Knowledge Neural Graphs
name = 'GFMult'
entity_embeddings
relation_embeddings
k
num_sample = 250
roots
weights

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

Parameters
x

class dicee.models.FMult2 (args)
Bases: dicee.models.base_model.BaseKGE
Learning Knowledge Neural Graphs
name = 'FMult2'
n_layers = 3
k
n = 50
score_func = 'compositional'
discrete_points

```

```

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

```

Parameters

x

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

Bases: *dicee.models.base_model.BaseKGE*

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

```

name = 'LFMult1'
entity_embeddings
relation_embeddings
forward_triples(idx_triple)

```

Parameters

x

tri_score(*h, r, t*)

vtp_score(*h, r, t*)

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

Bases: *dicee.models.base_model.BaseKGE*

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

```

name = 'LFMult'
entity_embeddings
relation_embeddings
degree
m
x_values

```

```

forward_triples (idx_triple)

Parameters
    x

construct_multi_coeff (x)

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

linear (x, w, b)

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

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

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

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

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

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

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

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

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

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

```

```
name = 'DualE'

entity_embeddings
relation_embeddings

num_ent = None

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

Input

x: torch.LongTensor with (n,) shape

Output

torch.FloatTensor with (n) shape

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

Negative Sampling forward pass:

Input

x: torch.LongTensor with (n,) shape

Output

torch.FloatTensor with (n) shape

```
forward_k_vs_all (x)
```

KvsAll forward pass

Input

x: torch.LongTensor with (n,) shape

Output

torch.FloatTensor with (n) shape

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

Transpose function

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

dicee.query_generator

Classes

```
QueryGenerator
```

Module Contents

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

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

```

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

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

abstract load_queries (path)

get_queries (query_type: str, gen_num: int)

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

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

```

dicee.read_preprocess_save_load_kg

Submodules

dicee.read_preprocess_save_load_kg.preprocess

Classes

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

Module Contents

```

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

    kg

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

```

Parameter

rtype	None
--------------	------

```

preprocess_with_byte_pair_encoding()

preprocess_with_byte_pair_encoding_with_padding() → None

preprocess_with_pandas() → None
    Preprocess train, valid and test datasets stored in knowledge graph instance with pandas
    (1) Add recipriocal or noisy triples
    (2) Construct vocabulary
    (3) Index datasets

```

Parameter

rtype

None

`preprocess_with_polars()` → None

`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

ReadFromDisk

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

LoadSaveToDisk

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)	
<code>read_with_polars</code> (→ polars.DataFrame) <code>read_with_pandas</code> (data_path[, read_only_few, ...])	Load and Preprocess via Polars
<code>read_from_disk</code> (→ Tuple[polars.DataFrame, pandas.DataFrame]) <code>read_from_triple_store</code> ([endpoint]) <code>get_er_vocab</code> (data[, file_path])	Read triples from triple store into pandas dataframe
<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) <code>save_numpy_ndarray</code> (*[, data, file_path])	Deserialize data
<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) <code>dataset_sanity_checking</code> (→ None)	Add inverse triples into dask dataframe

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*.

- 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)
```

- (1) Add reciprocal triples
- (2) Add noisy triples

```
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)
```

```
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.read_from_triple_store(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_pandas() → None
    Preprocess train, valid and test datasets stored in knowledge graph instance with pandas
        (1) Add reciprocical or noisy triples
        (2) Construct vocabulary
        (3) Index datasets

Parameter

rtype
    None

preprocess_with_polars() → None

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

<code>is_sparql_endpoint_alive([sparql_endpoint])</code>	
<code>validate_knowledge_graph(args)</code>	Validating the source of knowledge graph
<code>sanity_checking_with_arguments(args)</code>	
<code>sanity_check_callback_args(args)</code>	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`

!!! abstract "Usage Documentation"

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(/, **data: Any)  
Bases: pydantic.BaseModel  
  
!!! abstract “Usage Documentation”  
[Models](./concepts/models.md)  
  
A base class for creating Pydantic models.
```

`__class_vars__`
The names of the class variables defined on the model.

`__private_attributes__`
Metadata about the private attributes of the model.

`__signature__`
The synthesized `__init__` [Signature][inspect.Signature] of the model.

`__pydantic_complete__`
Whether model building is completed, or if there are still undefined fields.

`__pydantic_core_schema__`
The core schema of the model.

`__pydantic_custom_init__`
Whether the model has a custom `__init__` function.

`__pydantic_decorators__`
Metadata containing the decorators defined on the model. This replaces `Model.__validators__` and `Model.__root_validators__` from Pydantic V1.

`__pydantic_generic_metadata__`
Metadata for generic models; contains data used for a similar purpose to `__args__`, `__origin__`, `__parameters__` in typing-module generics. May eventually be replaced by these.

`__pydantic_parent_namespace__`
Parent namespace of the model, used for automatic rebuilding of models.

`__pydantic_post_init__`
The name of the post-init method for the model, if defined.

`__pydantic_root_model__`
Whether the model is a [RootModel][pydantic.root_model.RootModel].

`__pydantic_serializer__`
The *pydantic-core SchemaSerializer* used to dump instances of the model.

`__pydantic_validator__`
The *pydantic-core SchemaValidator* used to validate instances of the model.

`__pydantic_fields__`
A dictionary of field names and their corresponding [FieldInfo][pydantic.fields.FieldInfo] objects.

`__pydantic_computed_fields__`
A dictionary of computed field names and their corresponding [ComputedField-Info][pydantic.fields.ComputedFieldInfo] objects.

`__pydantic_extra__`
A dictionary containing extra values, if [extra][pydantic.config.ConfigDict.extra] is set to 'allow'.

`__pydantic_fields_set__`
The names of fields explicitly set during instantiation.

`__pydantic_private__`
Values of private attributes set on the model instance.

`queries: List[str]`

```

    reducer: str | None = None

async dicee.scripts.index_serve.search_embeddings_batch(request: StringListRequest)

dicee.scripts.index_serve.serve(args)

dicee.scripts.index_serve.main()

```

dicee.scripts.run

Functions

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

continues on next page

Table 2 – continued from previous page

<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>initialize_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>	

Module Contents

```
dicee.static_funcs.create_reciprocal_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*, ***kargs*)

Train model

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

trainer

local_rank

global_rank

```

optimizer
train_dataset_loader
loss_func
callbacks
model
num_epochs
loss_history = []
ctx
scaler
extract_input_outputs(z: list)
train()
    Training loop for DDP

```

Classes

<i>DICE_Trainer</i>	DICE_Trainer implement
---------------------	------------------------

Package Contents

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

DICE_Trainer implement

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

```

args
is_continual_training:bool
storage_path:str
evaluator:
report:dict

```

report

args

```

trainer = None
is_continual_training
storage_path
evaluator = None
form_of_labelling = None

```

```
continual_start (knowledge_graph)
```

- (1) Initialize training.
- (2) Load model
- (3) Load trainer (3) Fit model

Parameter

returns

- *model*
- **form_of_labelling** (*str*)

```
initialize_trainer (callbacks: List)
```

→ lightning.Trainer | dicee.trainer.model_parallelism.TensorParallel | dicee.trainer.torch_trainer.TorchTrainer | dicee.

Initialize Trainer from input arguments

```
initialize_or_load_model ()
```

```
init_dataloader (dataset: torch.utils.data.Dataset) → torch.utils.data.DataLoader
```

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

```
start (knowledge_graph: dicee.knowledge_graph.KG | numpy.memmap)
```

→ Tuple[dicee.models.base_model.BaseKGE, str]

Start the training

- (1) Initialize Trainer

- (2) Initialize or load a pretrained KGE model

in DDP setup, we need to load the memory map of already read/index KG.

```
k_fold_cross_validation (dataset) → Tuple[dicee.models.base_model.BaseKGE, str]
```

Perform K-fold Cross-Validation

1. Obtain K train and test splits.

2. **For each split,**

2.1 initialize trainer and model 2.2. Train model with configuration provided in args. 2.3. Compute the mean reciprocal rank (MRR) score of the model on the test respective split.

3. Report the mean and average MRR .

Parameters

- **self**
- **dataset**

Returns

model

14.2 Attributes

```
__version__
```

14.3 Classes

<i>Pyke</i>	A Physical Embedding Model for Knowledge Graphs
<i>DistMult</i>	Embedding Entities and Relations for Learning and Inference in Knowledge Bases
<i>CKeci</i>	Without learning dimension scaling
<i>Keci</i>	Base class for all neural network modules.
<i>TransE</i>	Translating Embeddings for Modeling
<i>DeCaL</i>	Base class for all neural network modules.
<i>Duale</i>	Dual Quaternion Knowledge Graph Embeddings (https://ojs.aaai.org/index.php/AAAI/article/download/16850/16657)
<i>ComplEx</i>	Base class for all neural network modules.
<i>AConEx</i>	Additive Convolutional ComplEx Knowledge Graph Embeddings
<i>AConvO</i>	Additive Convolutional Octonion Knowledge Graph Embeddings
<i>AConvQ</i>	Additive Convolutional Quaternion Knowledge Graph Embeddings
<i>ConvQ</i>	Convolutional Quaternion Knowledge Graph Embeddings
<i>Convo</i>	Base class for all neural network modules.
<i>ConEx</i>	Convolutional ComplEx Knowledge Graph Embeddings
<i>QMult</i>	Base class for all neural network modules.
<i>OMult</i>	Base class for all neural network modules.
<i>Shallom</i>	A shallow neural model for relation prediction (https://arxiv.org/abs/2101.09090)
<i>LFMult</i>	Embedding with polynomial functions. We represent all entities and relations in the polynomial space as:
<i>PykeenKGE</i>	A class for using knowledge graph embedding models implemented in Pykeen
<i>Byte</i>	Base class for all neural network modules.
<i>BaseKGE</i>	Base class for all neural network modules.
<i>EnsembleKGE</i>	
<i>DICE_Trainer</i>	DICE_Trainer implement
<i>KGE</i>	Knowledge Graph Embedding Class for interactive usage of pre-trained models
<i>Execute</i>	A class for Training, Retraining and Evaluation a model.
<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

continues on next page

Table 3 – continued from previous page

<i>CVDataModule</i>	Create a Dataset for cross validation
<i>LiteralDataset</i>	Dataset for loading and processing literal data for training
<i>QueryGenerator</i>	Literal Embedding model.

14.4 Functions

<i>create_reciprocal_triples</i> (x)	Add inverse triples into dask dataframe
<i>get_er_vocab</i> (data[, file_path])	
<i>get_re_vocab</i> (data[, file_path])	
<i>get_ee_vocab</i> (data[, file_path])	
<i>timeit</i> (func)	
<i>save_pickle</i> (*[, data, file_path])	
<i>load_pickle</i> ([file_path])	
<i>load_term_mapping</i> ([file_path])	
<i>select_model</i> (args[, is_continual_training, storage_path])	
<i>load_model</i> (→ Tuple[object, Tuple[dict, dict]])	Load weights and initialize pytorch module from namespace arguments
<i>load_model_ensemble</i> (...)	Construct Ensemble Of weights and initialize pytorch module from namespace arguments
<i>save_numpy_ndarray</i> (*[, data, file_path])	
<i>numpy_data_type_changer</i> (→ numpy.ndarray)	Detect most efficient data type for a given triples
<i>save_checkpoint_model</i> (→ None)	Store Pytorch model into disk
<i>store</i> (→ None)	
<i>add_noisy_triples</i> (→ pandas.DataFrame)	Add randomly constructed triples
<i>read_or_load_kg</i> (args, cls)	
<i>intialize_model</i> (→ Tuple[object, str])	
<i>load_json</i> (→ dict)	
<i>save_embeddings</i> (→ None)	Save it as CSV if memory allows.
<i>random_prediction</i> (pre_trained_kge)	
<i>deploy_triple_prediction</i> (pre_trained_kge, str_subject, ...)	
<i>deploy_tail_entity_prediction</i> (pre_trained_kge, ...)	

continues on next page

Table 4 – continued from previous page

<code>deploy_head_entity_prediction</code> (<code>pre_trained_kge</code> , ...)	
<code>deploy_relation_prediction</code> (<code>pre_trained_kge</code> , ...)	
<code>vocab_to_parquet</code> (<code>vocab_to_idx</code> , <code>name</code> , ...)	
<code>create_experiment_folder</code> ([<code>folder_name</code>])	
<code>continual_training_setup_executor</code> (→ <code>None</code>)	
<code>exponential_function</code> (→ <code>torch.FloatTensor</code>)	
<code>load_numpy</code> (→ <code>numpy.ndarray</code>)	
<code>evaluate</code> (<code>entity_to_idx</code> , <code>scores</code> , <code>easy_answers</code> , # @TODO: CD: Renamed this function <code>hard_answers</code>)	
<code>download_file</code> (<code>url</code> [, <code>destination_folder</code>])	
<code>download_files_from_url</code> (→ <code>None</code>)	
<code>download_pretrained_model</code> (→ <code>str</code>)	
<code>write_csv_from_model_parallel</code> (<code>path</code>)	Create
<code>from_pretrained_model_write_embeddings_int</code> (<code>None</code>)	
<code>mapping_from_first_two_cols_to_third</code> (<code>train_se</code>)	
<code>timeit</code> (<code>func</code>)	
<code>load_term_mapping</code> ([<code>file_path</code>])	
<code>reload_dataset</code> (<code>path</code> , <code>form_of_labelling</code> , ...)	Reload the files from disk to construct the Pytorch dataset
<code>construct_dataset</code> (→ <code>torch.utils.data.Dataset</code>)	

14.5 Package Contents

```
class dicee.Pyke(args)
    Bases: dicee.models.base_model.BaseKGE
    A Physical Embedding Model for Knowledge Graphs
    name = 'Pyke'
    dist_func
    margin = 1.0
    forward_triples(x: torch.LongTensor)
```

Parameters

`x`

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

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

```
name = 'DistMult'

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

Parameters

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

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

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

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

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

Bases: `Keci`

Without learning dimension scaling

```
name = 'CKeci'
```

```
requires_grad_for_interactions = False
```

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

Bases: `dicee.models.base_model.BaseKGE`

Base class for all neural network modules.

Your models should also subclass this class.

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

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

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

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

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

Note

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

Variables

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

```
name = 'Keci'

p
q
r

requires_grad_for_interactions = True

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

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

e2e1, e2e2, e2e3, e3e1, e3e2, e3e3

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

```
compute_sigma_qq(hq, rq)
    Compute sigma_{qq} = sum_{j=1}^{p+q-1} sum_{k=j+1}^{p+q} (h_j r_k - h_k r_j) e_j e_k sigma_{q}
    sigma_{qq} captures the interactions between along q bases For instance, let q e_1, e_2, e_3, we compute interactions
    between e_1 e_2, e_1 e_3 , and e_2 e_3 This can be implemented with a nested two for loops
```

results = [] for j in range(q - 1):
 for k in range(j + 1, q):
 results.append(hq[:, :, j] * rq[:, :, k] - hq[:, :, k] * rq[:, :, j])
 sigma_qq = torch.stack(results, dim=2) assert sigma_qq.shape == (b, r, int((q * (q - 1)) / 2))

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

e2e1, e2e2, e2e3, e3e1, e3e2, e3e3

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

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

```

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

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

clifford_multiplication (h0, hp, hq, r0, rp, rq)
    Compute our CL multiplication
        h = h_0 + sum_{i=1}^p h_i e_i + sum_{j=p+1}^{p+q} h_j e_j
        r = r_0 + sum_{i=1}^p r_i e_i +
        sum_{j=p+1}^{p+q} r_j e_j
        ei ^2 = +1 for i <= p ej ^2 = -1 for p < j <= p+q ei ej = -eje1 for i
        eq j
        h r = sigma_0 + sigma_p + sigma_q + sigma_{pp} + sigma_{q} + sigma_{pq} where
        (1) sigma_0 = h_0 r_0 + sum_{i=1}^p (h_0 r_i) e_i - sum_{j=p+1}^{p+q} (h_j r_j) e_j
        (2) sigma_p = sum_{i=1}^p (h_0 r_i + h_i r_0) e_i
        (3) sigma_q = sum_{j=p+1}^{p+q} (h_0 r_j + h_j r_0) e_j
        (4) sigma_{pp} = sum_{i=1}^{p-1} sum_{k=i+1}^p (h_i r_k - h_k r_i) e_i e_k
        (5) sigma_{qq} = sum_{j=1}^{p+q-1} sum_{k=j+1}^{p+q} (h_j r_k - h_k r_j) e_j e_k
        (6) sigma_{pq} = sum_{i=1}^p sum_{j=p+1}^{p+q} (h_i r_j - h_j r_i) e_i e_j

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

```

Parameter

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

returns

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

forward_k_vs_with_explicit (x: torch.Tensor)

k_vs_all_score (bpe_head_ent_emb, bpe_rel_ent_emb, E)

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

Kvsall training

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

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

```
construct_batch_selected_cl_multivector(x: torch.FloatTensor, r: int, p: int, q: int)
    → tuple[torch.FloatTensor, torch.FloatTensor, torch.FloatTensor]
```

Construct a batch of batchs multivectors $\text{Cl}_{\{p,q\}}(\mathbb{R}^d)$

Parameter

x: torch.FloatTensor with (n,k, d) shape

returns

- **a0** (torch.FloatTensor with (n, k, m) shape)
- **ap** (torch.FloatTensor with (n, k, m, p) shape)
- **aq** (torch.FloatTensor with (n, k, m, q) shape)

```
forward_k_vs_sample(x: torch.LongTensor, target_entity_idx: torch.LongTensor) → torch.FloatTensor
```

Parameter

x: torch.LongTensor with (n,2) shape

target_entity_idx: torch.LongTensor with (n, k) shape k denotes the selected number of examples.

rtype

torch.FloatTensor with (n, k) shape

```
score(h, r, t)
```

```
forward_triples(x: torch.Tensor) → torch.FloatTensor
```

Parameter

x: torch.LongTensor with (n,3) shape

rtype

torch.FloatTensor with (n) shape

```
class dicee.TransE(args)
```

Bases: *dicee.models.base_model.BaseKGE*

Translating Embeddings for Modeling Multi-relational Data <https://proceedings.neurips.cc/paper/2013/file/1cecc7a77928ca8133fa24680a88d2f9-Paper.pdf>

```
name = 'TransE'
```

```
margin = 4
```

```
score(head_ent_emb, rel_ent_emb, tail_ent_emb)
```

```
forward_k_vs_all(x: torch.Tensor) → torch.FloatTensor
```

```
class dicee.DeCaL(args)
```

Bases: *dicee.models.base_model.BaseKGE*

Base class for all neural network modules.

Your models should also subclass this class.

Modules can also contain other Modules, allowing them to be nested in a tree structure. You can assign the sub-modules as regular attributes:

```

import torch.nn as nn
import torch.nn.functional as F

class Model(nn.Module):
    def __init__(self) -> None:
        super().__init__()
        self.conv1 = nn.Conv2d(1, 20, 5)
        self.conv2 = nn.Conv2d(20, 20, 5)

    def forward(self, x):
        x = F.relu(self.conv1(x))
        return F.relu(self.conv2(x))

```

Submodules assigned in this way will be registered, and will also have their parameters converted when you call `to()`, etc.

Note

As per the example above, an `__init__()` call to the parent class must be made before assignment on the child.

Variables

`training (bool)` – Boolean represents whether this module is in training or evaluation mode.

```

name = 'DeCaL'

entity_embeddings

relation_embeddings

p

q

r

re

forward_triples(x: torch.Tensor) → torch.FloatTensor

```

Parameter

`x: torch.LongTensor with (n,) shape`

`rtype`

`torch.FloatTensor with (n) shape`

`c1_pqr(a: torch.tensor) → torch.tensor`

Input: tensor(batch_size, emb_dim) —> output: tensor with 1+p+q+r components with size (batch_size, emb_dim/(1+p+q+r)) each.

1) takes a tensor of size (batch_size, emb_dim), split it into 1 + p + q +r components, hence 1+p+q+r must be a divisor of the emb_dim. 2) Return a list of the 1+p+q+r components vectors, each are tensors of size (batch_size, emb_dim/(1+p+q+r))

compute_sigmas_single (*list_h_emb*, *list_r_emb*, *list_t_emb*)

here we compute all the sums with no others vectors interaction taken with the scalar product with t, that is,

$$s0 = h_0 r_0 t_0 s1 = \sum_{i=1}^p h_i r_i t_0 s2 = \sum_{j=p+1}^{p+q} h_j r_j t_0 s3 = \sum_{i=1}^q (h_0 r_i t_i + h_i r_0 t_i) s4 = \sum_{i=p+1}^{p+q} (h_0 r_i t_i + h_i r_0 t_i) s5 = \sum_{i=p+q+1}^{p+q+r} (h_0 r_i t_i + h_i r_0 t_i)$$

and return:

$$\text{sigma}_0 t = \sigma_0 \cdot t_0 = s0 + s1 - s2s3, s4 \text{ and } s5$$

compute_sigmas_multivect (*list_h_emb*, *list_r_emb*)

Here we compute and return all the sums with vectors interaction for the same and different bases.

For same bases vectors interaction we have

$$\sigma_p p = \sum_{i=1}^{p-1} \sum_{i'=i+1}^p (h_i r_{i'} - h_{i'} r_i) \text{ (models the interactions between } e_i \text{ and } e'_{i'} \text{ for } 1 \leq i, i' \leq p) \sigma_q q = \sum_{j=p+1}^{p+q-1} \sum_{j'=j+1}^{p+q} (h_j r_{j'} - h_{j'} r_j) \text{ (interactions between } e_i \text{ and } e_j \text{ for } 1 \leq i \leq p \text{ and } p+1 \leq j \leq p+q) \sigma_p r = \sum_{i=1}^p (h_i r_i - h_i r_i)$$

For different base vector interactions, we have

$$\sigma_p q = \sum_{i=1}^p \sum_{j=p+1}^{p+q} (h_i r_j - h_j r_i) \text{ (interactions between } e_i \text{ and } e_j \text{ for } 1 \leq i \leq p \text{ and } p+1 \leq j \leq p+q) \sigma_p r = \sum_{i=1}^p (h_i r_i - h_i r_i)$$

forward_k_vs_all (*x*: *torch.Tensor*) → *torch.FloatTensor*

Kvsall training

- (1) Retrieve real-valued embedding vectors for heads and relations
- (2) Construct head entity and relation embeddings according to $\text{Cl}_{\{p,q,r\}}(\mathbb{R}^d)$.
- (3) Perform Cl multiplication
- (4) Inner product of (3) and all entity embeddings

forward_k_vs_with_explicit and this funcitons are identical Parameter ——— *x*: *torch.LongTensor* with (n,) shape :rtype: *torch.FloatTensor* with (n, |E|) shape

apply_coefficients (*h0*, *hp*, *hq*, *hk*, *r0*, *rp*, *rq*, *rk*)

Multiplying a base vector with its scalar coefficient

construct_cl_multivector (*x*: *torch.FloatTensor*, *re*: int, *p*: int, *q*: int, *r*: int)

→ tuple[*torch.FloatTensor*, *torch.FloatTensor*, *torch.FloatTensor*]

Construct a batch of multivectors $\text{Cl}_{\{p,q,r\}}(\mathbb{R}^d)$

Parameter

x: *torch.FloatTensor* with (n,d) shape

returns

- **a0** (*torch.FloatTensor*)
- **ap** (*torch.FloatTensor*)
- **aq** (*torch.FloatTensor*)
- **ar** (*torch.FloatTensor*)

```
compute_sigma_pp(hp, rp)
```

Compute .. math:

$$\sigma_{p,p}^* = \sum_{i=1}^{p-1} \sum_{i'=i+1}^p (x_i y_{i'} - x_{i'} y_i)$$

$\sigma_{p,p}$ captures the interactions between along p bases For instance, let $p = 1, 2, 3$, we compute interactions between $e_1 e_2, e_1 e_3, e_2 e_3$. This can be implemented with a nested two for loops

results = [] for i in range(p - 1):

```
for k in range(i + 1, p):
```

```
    results.append(hp[:, :, i] * rp[:, :, k] - hp[:, :, k] * rp[:, :, i])
```

```
sigma_pp = torch.stack(results, dim=2) assert sigma_pp.shape == (b, r, int((p * (p - 1)) / 2))
```

Yet, this computation would be quite inefficient. Instead, we compute interactions along all p, e.g., $e_1 e_1, e_1 e_2, e_1 e_3, e_2 e_1, e_2 e_2, e_2 e_3, e_3 e_1, e_3 e_2, e_3 e_3$

Then select the triangular matrix without diagonals: $e_1 e_2, e_1 e_3, e_2 e_3$.

```
compute_sigma_qq(hq, rq)
```

Compute

$$\sigma_{q,q}^* = \sum_{j=p+1}^{p+q-1} \sum_{j'=j+1}^{p+q} (x_j y_{j'} - x_{j'} y_j) Eq.16$$

$\sigma_{q,q}$ captures the interactions between along q bases For instance, let $q = 1, 2, 3$, we compute interactions between $e_1 e_2, e_1 e_3, e_2 e_3$. This can be implemented with a nested two for loops

results = [] for j in range(q - 1):

```
for k in range(j + 1, q):
```

```
    results.append(hq[:, :, j] * rq[:, :, k] - hq[:, :, k] * rq[:, :, j])
```

```
sigma_qq = torch.stack(results, dim=2) assert sigma_qq.shape == (b, r, int((q * (q - 1)) / 2))
```

Yet, this computation would be quite inefficient. Instead, we compute interactions along all p, e.g., $e_1 e_1, e_1 e_2, e_1 e_3, e_2 e_1, e_2 e_2, e_2 e_3, e_3 e_1, e_3 e_2, e_3 e_3$

e2e1, e2e2, e2e3, e3e1, e3e2, e3e3

Then select the triangular matrix without diagonals: $e_1 e_2, e_1 e_3, e_2 e_3$.

```
compute_sigma_rr(hk, rk)
```

$$\sigma_{r,r}^* = \sum_{k=p+q+1}^{p+q+r-1} \sum_{k'=k+1}^p (x_k y_{k'} - x_{k'} y_k)$$

```
compute_sigma_pq(* , hp, hq, rp, rq)
```

Compute

$$\sum_{i=1}^p \sum_{j=p+1}^{p+q} (h_i r_j - h_j r_i) e_i e_j$$

results = [] sigma_pq = torch.zeros(b, r, p, q) for i in range(p):

```
for j in range(q):
```

```
    sigma_pq[:, :, i, j] = hp[:, :, i] * rq[:, :, j] - hq[:, :, j] * rp[:, :, i]
```

```

print(sigma_pq.shape)

compute_sigma_pr(*hp, hk, rp, rk)
    Compute

$$\sum_{i=1}^p \sum_{j=p+1}^{p+q} (h_i r_j - h_j r_i) e_i e_j$$

results = [] sigma_pq = torch.zeros(b, r, p, q) for i in range(p):
    for j in range(q):
        sigma_pq[:, :, i, j] = hp[:, :, i] * rq[:, :, j] - hk[:, :, j] * rp[:, :, i]
    print(sigma_pq.shape)

compute_sigma_qr(*hq, hk, rq, rk)

$$\sum_{i=1}^p \sum_{j=p+1}^{p+q} (h_i r_j - h_j r_i) e_i e_j$$

results = [] sigma_pq = torch.zeros(b, r, p, q) for i in range(p):
    for j in range(q):
        sigma_pq[:, :, i, j] = hp[:, :, i] * rq[:, :, j] - hk[:, :, j] * rp[:, :, i]
    print(sigma_pq.shape)

class dicee.Duale(args)
Bases: dicee.models.base_model.BaseKGE

Dual Quaternion Knowledge Graph Embeddings (https://ojs.aaai.org/index.php/AAAI/article/download/16850/16657)
    name = 'DualE'

    entity_embeddings
    relation_embeddings
    num_ent = None

    kvsall_score(e_1_h, e_2_h, e_3_h, e_4_h, e_5_h, e_6_h, e_7_h, e_8_h, e_1_t, e_2_t, e_3_t, e_4_t,
                  e_5_t, e_6_t, e_7_t, e_8_t, r_1, r_2, r_3, r_4, r_5, r_6, r_7, r_8) → torch.tensor
        KvsAll scoring function

```

Input

x: torch.LongTensor with (n,) shape

Output

torch.FloatTensor with (n) shape

forward_triples(idx_triple: torch.tensor) → torch.tensor

Negative Sampling forward pass:

Input

x: torch.LongTensor with (n,) shape

Output

torch.FloatTensor with (n) shape

```
forward_k_vs_all(x)
```

KvsAll forward pass

Input

x: torch.LongTensor with (n,) shape

Output

torch.FloatTensor with (n) shape

```
T(x: torch.tensor) → torch.tensor
```

Transpose function

Input: Tensor with shape (nxm) Output: Tensor with shape (mxn)

```
class dicee.Complex(args)
```

Bases: dicee.models.base_model.BaseKGE

Base class for all neural network modules.

Your models should also subclass this class.

Modules can also contain other Modules, allowing them to be nested in a tree structure. You can assign the sub-modules as regular attributes:

```
import torch.nn as nn
import torch.nn.functional as F

class Model(nn.Module):
    def __init__(self) -> None:
        super().__init__()
        self.conv1 = nn.Conv2d(1, 20, 5)
        self.conv2 = nn.Conv2d(20, 20, 5)

    def forward(self, x):
        x = F.relu(self.conv1(x))
        return F.relu(self.conv2(x))
```

Submodules assigned in this way will be registered, and will also have their parameters converted when you call `to()`, etc.

Note

As per the example above, an `__init__()` call to the parent class must be made before assignment on the child.

Variables

`training (bool)` – Boolean represents whether this module is in training or evaluation mode.

```
name = 'ComplEx'

static score(head_ent_emb: torch.FloatTensor, rel_ent_emb: torch.FloatTensor,
            tail_ent_emb: torch.FloatTensor)

static k_vs_all_score(emb_h: torch.FloatTensor, emb_r: torch.FloatTensor,
                      emb_E: torch.FloatTensor)
```

Parameters

- `emb_h`
- `emb_r`
- `emb_E`

`forward_k_vs_all(x: torch.LongTensor) → torch.FloatTensor`

`forward_k_vs_sample(x: torch.LongTensor, target_entity_idx: torch.LongTensor)`

`class dicee.AConEx(args)`

Bases: `dicee.models.base_model.BaseKGE`

Additive Convolutional ComplEx Knowledge Graph Embeddings

`name = 'AConEx'`

`conv2d`

`fc_num_input`

`fc1`

`norm_fc1`

`bn_conv2d`

`feature_map_dropout`

`residual_convolution(C_1: Tuple[torch.Tensor, torch.Tensor],
 C_2: Tuple[torch.Tensor, torch.Tensor]) → torch.FloatTensor`

Compute residual score of two complex-valued embeddings. :param C_1: a tuple of two pytorch tensors that corresponds complex-valued embeddings :param C_2: a tuple of two pytorch tensors that corresponds complex-valued embeddings :return:

`forward_k_vs_all(x: torch.Tensor) → torch.FloatTensor`

`forward_triples(x: torch.Tensor) → torch.FloatTensor`

Parameters

`x`

`forward_k_vs_sample(x: torch.Tensor, target_entity_idx: torch.Tensor)`

`class dicee.ACOnvo(args: dict)`

Bases: `dicee.models.base_model.BaseKGE`

Additive Convolutional Octonion Knowledge Graph Embeddings

```

name = 'AConvO'

conv2d

fc_num_input

fc1

bn_conv2d

norm_fc1

feature_map_dropout

static octonion_normalizer(emb_rel_e0, emb_rel_e1, emb_rel_e2, emb_rel_e3, emb_rel_e4,
                           emb_rel_e5, emb_rel_e6, emb_rel_e7)

residual_convolution(O_1, O_2)

forward_triples(x: torch.Tensor) → torch.Tensor

```

Parameters

x

forward_k_vs_all(x: torch.Tensor)

Given a head entity and a relation (h,r), we compute scores for all entities. [score(h,r,x)|x in Entities] => [0.0,0.1,...,0.8], shape=> (1, |Entities|) Given a batch of head entities and relations => shape (size of batch,|Entities|)

```

class dicee.AConvQ(args)

```

Bases: *dicee.models.base_model.BaseKGE*

Additive Convolutional Quaternion Knowledge Graph Embeddings

```

name = 'AConvQ'

```

```

entity_embeddings

```

```

relation_embeddings

```

```

conv2d

```

```

fc_num_input

```

```

fc1

```

```

bn_conv1

```

```

bn_conv2

```

```

feature_map_dropout

```

```

residual_convolution(Q_1, Q_2)

```

```

forward_triples(indexed_triple: torch.Tensor) → torch.Tensor

```

Parameters

x

```

forward_k_vs_all(x: torch.Tensor)
    Given a head entity and a relation (h,r), we compute scores for all entities. [score(h,r,x)|x in Entities] => [0.0,0.1,...,0.8], shape=>(1, |Entities|) Given a batch of head entities and relations => shape (size of batch,|Entities|)

class dicee.ConvQ(args)
    Bases: dicee.models.base_model.BaseKGE
    Convolutional Quaternion Knowledge Graph Embeddings
    name = 'ConvQ'

    entity_embeddings
    relation_embeddings
    conv2d
    fc_num_input
    fc1
    bn_conv1
    bn_conv2
    feature_map_dropout
    residual_convolution(Q_1, Q_2)

    forward_triples(indexed_triple: torch.Tensor) → torch.Tensor

```

Parameters

x

```
forward_k_vs_all(x: torch.Tensor)
```

Given a head entity and a relation (h,r), we compute scores for all entities. [score(h,r,x)|x in Entities] => [0.0,0.1,...,0.8], shape=>(1, |Entities|) Given a batch of head entities and relations => shape (size of batch,|Entities|)

```

class dicee.ConvO(args: dict)
    Bases: dicee.models.base_model.BaseKGE

```

Base class for all neural network modules.

Your models should also subclass this class.

Modules can also contain other Modules, allowing them to be nested in a tree structure. You can assign the sub-modules as regular attributes:

```

import torch.nn as nn
import torch.nn.functional as F

class Model(nn.Module):
    def __init__(self) -> None:
        super().__init__()
        self.conv1 = nn.Conv2d(1, 20, 5)
        self.conv2 = nn.Conv2d(20, 20, 5)

```

(continues on next page)

```
def forward(self, x):
    x = F.relu(self.conv1(x))
    return F.relu(self.conv2(x))
```

Submodules assigned in this way will be registered, and will also have their parameters converted when you call `to()`, etc.

Note

As per the example above, an `__init__()` call to the parent class must be made before assignment on the child.

Variables

`training (bool)` – Boolean represents whether this module is in training or evaluation mode.

```
name = 'Conv0'

conv2d

fc_num_input

fc1

bn_conv2d

norm_fc1

feature_map_dropout

static octonion_normalizer(emb_rel_e0, emb_rel_e1, emb_rel_e2, emb_rel_e3, emb_rel_e4,
                           emb_rel_e5, emb_rel_e6, emb_rel_e7)

residual_convolution(O_1, O_2)

forward_triples(x: torch.Tensor) → torch.Tensor
```

Parameters

`x`

`forward_k_vs_all(x: torch.Tensor)`

Given a head entity and a relation (h,r), we compute scores for all entities. [score(h,r,x)|x in Entities] => [0.0,0.1,...,0.8], shape=> (1, |Entities|) Given a batch of head entities and relations => shape (size of batch,|Entities|)

`class dicee.ConEx(args)`

Bases: `dicee.models.base_model.BaseKGE`

Convolutional ComplEx Knowledge Graph Embeddings

`name = 'ConEx'`

`conv2d`

`fc_num_input`

```

fc1
norm_fc1
bn_conv2d
feature_map_dropout

residual_convolution(C_1: Tuple[torch.Tensor, torch.Tensor],  

C_2: Tuple[torch.Tensor, torch.Tensor]) → torch.FloatTensor
    Compute residual score of two complex-valued embeddings. :param C_1: a tuple of two pytorch tensors  

    that corresponds complex-valued embeddings :param C_2: a tuple of two pytorch tensors that corresponds  

    complex-valued embeddings :return:
forward_k_vs_all(x: torch.Tensor) → torch.FloatTensor
forward_triples(x: torch.Tensor) → torch.FloatTensor

Parameters
    x
forward_k_vs_sample(x: torch.Tensor, target_entity_idx: torch.Tensor)

class dicee.QMult(args)
    Bases: dicee.models.base_model.BaseKGE
    Base class for all neural network modules.
    Your models should also subclass this class.
    Modules can also contain other Modules, allowing them to be nested in a tree structure. You can assign the sub-
    modules as regular attributes:

    import torch.nn as nn
    import torch.nn.functional as F

    class Model(nn.Module):
        def __init__(self) -> None:
            super().__init__()
            self.conv1 = nn.Conv2d(1, 20, 5)
            self.conv2 = nn.Conv2d(20, 20, 5)

        def forward(self, x):
            x = F.relu(self.conv1(x))
            return F.relu(self.conv2(x))

```

Submodules assigned in this way will be registered, and will also have their parameters converted when you call `to()`, etc.

Note

As per the example above, an `__init__()` call to the parent class must be made before assignment on the child.

Variables

`training` (`bool`) – Boolean represents whether this module is in training or evaluation mode.

```

name = 'QMult'
explicit = True
quaternion_multiplication_followed_by_inner_product(h, r, t)

```

Parameters

- **h** – shape: (*batch_dims, dim) The head representations.
- **r** – shape: (*batch_dims, dim) The head representations.
- **t** – shape: (*batch_dims, dim) The tail representations.

Returns

Triple scores.

```
static quaternion_normalizer(x: torch.FloatTensor) → torch.FloatTensor
```

Normalize the length of relation vectors, if the forward constraint has not been applied yet.

Absolute value of a quaternion

$$|a + bi + cj + dk| = \sqrt{a^2 + b^2 + c^2 + d^2}$$

L2 norm of quaternion vector:

$$\|x\|^2 = \sum_{i=1}^d |x_i|^2 = \sum_{i=1}^d (x_i.re^2 + x_i.im_1^2 + x_i.im_2^2 + x_i.im_3^2)$$

Parameters

x – The vector.

Returns

The normalized vector.

```
score(head_ent_emb: torch.FloatTensor, rel_ent_emb: torch.FloatTensor,
      tail_ent_emb: torch.FloatTensor)
```

```
k_vs_all_score(bpe_head_ent_emb, bpe_rel_ent_emb, E)
```

Parameters

- **bpe_head_ent_emb**
- **bpe_rel_ent_emb**
- **E**

```
forward_k_vs_all(x)
```

Parameters

x

```
forward_k_vs_sample(x, target_entity_idx)
```

Completed. Given a head entity and a relation (h,r), we compute scores for all possible triples,i.e., [score(h,r,x)|x in Entities] => [0.0,0.1,...,0.8], shape=> (1, |Entities|) Given a batch of head entities and relations => shape (size of batch,| Entities|)

```
class dicee.OMult(args)
Bases: dicee.models.base_model.BaseKGE
```

Base class for all neural network modules.

Your models should also subclass this class.

Modules can also contain other Modules, allowing them to be nested in a tree structure. You can assign the sub-modules as regular attributes:

```
import torch.nn as nn
import torch.nn.functional as F

class Model(nn.Module):
    def __init__(self) -> None:
        super().__init__()
        self.conv1 = nn.Conv2d(1, 20, 5)
        self.conv2 = nn.Conv2d(20, 20, 5)

    def forward(self, x):
        x = F.relu(self.conv1(x))
        return F.relu(self.conv2(x))
```

Submodules assigned in this way will be registered, and will also have their parameters converted when you call `to()`, etc.

Note

As per the example above, an `__init__()` call to the parent class must be made before assignment on the child.

Variables

`training(bool)` – Boolean represents whether this module is in training or evaluation mode.

```
name = 'OMult'

static octonion_normalizer(emb_rel_e0, emb_rel_e1, emb_rel_e2, emb_rel_e3, emb_rel_e4,
emb_rel_e5, emb_rel_e6, emb_rel_e7)

score(head_ent_emb: torch.FloatTensor, rel_ent_emb: torch.FloatTensor,
tail_ent_emb: torch.FloatTensor)

k_vs_all_score(bpe_head_ent_emb, bpe_rel_ent_emb, E)
```

`forward_k_vs_all(x)`

Completed. Given a head entity and a relation (h,r), we compute scores for all possible triples,i.e., [score(h,r,x)|x in Entities] => [0.0,0.1,...,0.8], shape=>(1, |Entities|) Given a batch of head entities and relations => shape (size of batch,| Entities|)

```
class dicee.Shallom(args)
```

Bases: dicee.models.base_model.BaseKGE

A shallow neural model for relation prediction (<https://arxiv.org/abs/2101.09090>)

```
name = 'Shallom'
```

```

shallom

get_embeddings() → Tuple[numpy.ndarray, None]

forward_k_vs_all(x) → torch.FloatTensor

forward_triples(x) → torch.FloatTensor

    Parameters
        x

    Returns

class dicee.LFMult(args)
Bases: dicee.models.base_model.BaseKGE

Embedding with polynomial functions. We represent all entities and relations in the polynomial space as:  $f(x) = \sum_{i=0}^{d-1} a_k x^{i \% d}$  and use the three different scoring function as in the paper to evaluate the score. We also consider combining with Neural Networks.

name = 'LFMult'

entity_embeddings

relation_embeddings

degree

m

x_values

forward_triples(idx_triple)

    Parameters
        x

construct_multi_coeff(x)

poly_NN(x, coefh, coefr, coeft)
Constructing a 2 layers NN to represent the embeddings.  $h = \sigma(w_h^T x + b_h)$ ,  $r = \sigma(w_r^T x + b_r)$ ,  $t = \sigma(w_t^T x + b_t)$ 

linear(x, w, b)

scalar_batch_NN(a, b, c)
element wise multiplication between a,b and c: Inputs : a, b, c =====> torch.tensor of size batch_size x m x d Output : a tensor of size batch_size x d

tri_score(coeff_h, coeff_r, coeff_t)
this part implement the trilinear scoring techniques:

$$\text{score}(h, r, t) = \int_0^1 h(x)r(x)t(x) dx = \sum_{i,j,k=0}^{d-1} \frac{a_i b_j c_k}{(i+j+k+1)^d}$$


1. generate the range for i,j and k from [0 d-1]
2. perform  $\frac{a_i b_j c_k}{(i+j+k+1)^d}$  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 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

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 = 'ByteE'

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: `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.EnsembleKGE (seed_model=None, pretrained_models: List = None)

name

```

```

train_mode = True
named_children()
property example_input_array
parameters()
modules()

__iter__()
__len__()
eval()
to(device)
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

class dicee.**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

args**is_continual_training = False****trainer = None****trained_model = None****knowledge_graph = None****report****evaluator = None****start_time = None****setup_executor()** → None**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

```

dicee.mapping_from_first_two_cols_to_third(train_set_idx)

dicee.timeit(func)

dicee.load_term_mapping(file_path=str)

dicee.reload_dataset(path: str, form_of_labelling, scoring_technique, neg_ratio, label_smoothing_rate)
    Reload the files from disk to construct the Pytorch dataset

dicee.construct_dataset(*,
    train_set: numpy.ndarray | list, valid_set=None, test_set=None,
    ordered_bpe_entities=None, train_target_indices=None, target_dim: int = None, entity_to_idx: dict,
    relation_to_idx: dict, form_of_labelling: str, scoring_technique: str, neg_ratio: int,
    label_smoothing_rate: float, byte_pair_encoding=None, block_size: int = None)
    → torch.utils.data.Dataset

```

```

class dicee.BPE_NegativeSamplingDataset(train_set: torch.LongTensor,
    ordered_shaped_bpe_entities: torch.LongTensor, neg_ratio: int)

```

Bases: torch.utils.data.Dataset

An abstract class representing a Dataset.

All datasets that represent a map from keys to data samples should subclass it. All subclasses should overwrite `__getitem__()`, supporting fetching a data sample for a given key. Subclasses could also optionally overwrite `__len__()`, which is expected to return the size of the dataset by many Sampler implementations and the default options of DataLoader. Subclasses could also optionally implement `__getitems__()`, for speedup batched samples loading. This method accepts list of indices of samples of batch and returns list of samples.

Note

`Dataloader` by default constructs an index sampler that yields integral indices. To make it work with a map-style dataset with non-integral indices/keys, a custom sampler must be provided.

```

train_set
ordered_bpe_entities
num_bpe_entities
neg_ratio
num_datapoints
__len__()

```

```

__getitem__(idx)

collate_fn(batch_shaped_bpe_triples: List[Tuple[torch.Tensor, torch.Tensor]])
```

class dicee.**MultiLabelDataset** (train_set: *torch.LongTensor*, train_indices_target: *torch.LongTensor*,
 target_dim: *int*, torch_ordered_shaped_bpe_entities: *torch.LongTensor*)

Bases: *torch.utils.data.Dataset*

An abstract class representing a Dataset.

All datasets that represent a map from keys to data samples should subclass it. All subclasses should overwrite `__getitem__()`, supporting fetching a data sample for a given key. Subclasses could also optionally overwrite `__len__()`, which is expected to return the size of the dataset by many `Sampler` implementations and the default options of `DataLoader`. Subclasses could also optionally implement `__getitems__()`, for speedup batched samples loading. This method accepts list of indices of samples of batch and returns list of samples.

Note

`DataLoader` by default constructs an index sampler that yields integral indices. To make it work with a map-style dataset with non-integral indices/keys, a custom sampler must be provided.

```

train_set

train_indices_target

target_dim

num_datapoints

torch_ordered_shaped_bpe_entities

collate_fn = None

__len__()

__getitem__(idx)

class dicee.MultiClassClassificationDataset (subword_units: numpy.ndarray, block_size: int = 8)
```

Bases: *torch.utils.data.Dataset*

Dataset for the 1vsALL training strategy

Parameters

- `train_set_idx` – Indexed triples for the training.
- `entity_idxs` – mapping.
- `relation_idxs` – mapping.
- `form` – ?
- `num_workers` – *int* for <https://pytorch.org/docs/stable/data.html#torch.utils.data.DataLoader>

Return type

torch.utils.data.Dataset

`train_data`

```

block_size = 8

num_of_data_points

collate_fn = None

__len__()

__getitem__(idx)

class dicee.OnevsAllDataset(train_set_idx: numpy.ndarray, entity_idxs)

```

Bases: torch.utils.data.Dataset

Dataset for the 1vsALL training strategy

Parameters

- **train_set_idx** – Indexed triples for the training.
- **entity_idxs** – mapping.
- **relation_idxs** – mapping.
- **form** – ?
- **num_workers** – int for <https://pytorch.org/docs/stable/data.html#torch.utils.data.DataLoader>

Return type

torch.utils.data.Dataset

```

train_data

target_dim

collate_fn = None

__len__()

__getitem__(idx)

class dicee.KvsAll(train_set_idx: numpy.ndarray, entity_idxs, relation_idxs, form, store=None,
label_smoothing_rate: float = 0.0)

```

Bases: torch.utils.data.Dataset

Creates a dataset for KvsAll training by inheriting from torch.utils.data.Dataset.

Let D denote a dataset for KvsAll training and be defined as $D := \{(x,y)_i\}_{i=1}^N$, where $x: (h,r)$ is 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 $[0,1]^{\{|\mathcal{E}|\}}$ 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 $[0,1]^{|E|}$ which is a binary label.

overall $y_{i,j} = 1$ s.t. $(h, r) \in E_i$ in KG

Note

AllvsAll extends KvsAll via none existing (h,r). Hence, it adds data points that are labelled without 1s, only with 0s.

train_set_idx
 [numpy.ndarray] n by 3 array representing n triples
entity_idxs
 [dictionary] string representation of an entity to its integer id
relation_idxs
 [dictionary] string representation of a relation to its integer id

self : torch.utils.data.Dataset

```
>>> a = AllvsAll()
>>> a
? array([0, 1, 2, 3, 4, 5, 6, 7, 8, 9])
```

train_data = None
train_target = None

```

label_smoothing_rate
collate_fn = None
target_dim
__len__()
__getitem__(idx)

class dicee.OnevsSample(train_set: numpy.ndarray, num_entities, num_relations,
                      neg_sample_ratio: int = None, label_smoothing_rate: float = 0.0)
Bases: torch.utils.data.Dataset

```

A custom PyTorch Dataset class for knowledge graph embeddings, which includes both positive and negative sampling for a given dataset for multi-class classification problem..

Parameters

- **train_set** (*np.ndarray*) – A numpy array containing triples of knowledge graph data. Each triple consists of (head_entity, relation, tail_entity).
- **num_entities** (*int*) – The number of unique entities in the knowledge graph.
- **num_relations** (*int*) – The number of unique relations in the knowledge graph.
- **neg_sample_ratio** (*int, optional*) – The number of negative samples to be generated per positive sample. Must be a positive integer and less than num_entities.
- **label_smoothing_rate** (*float, optional*) – A label smoothing rate to apply to the positive and negative labels. Defaults to 0.0.

train_data

The input data converted into a PyTorch tensor.

Type

torch.Tensor

num_entities

Number of entities in the dataset.

Type

int

num_relations

Number of relations in the dataset.

Type

int

neg_sample_ratio

Ratio of negative samples to be drawn for each positive sample.

Type

int

label_smoothing_rate

The smoothing factor applied to the labels.

Type

torch.Tensor

collate_fn
A function that can be used to collate data samples into batches (set to None by default).

Type
function, optional

train_data

num_entities

num_relations

neg_sample_ratio = None

label_smoothing_rate

collate_fn = None

__len__()

Returns the number of samples in the dataset.

__getitem__(idx)

Retrieves a single data sample from the dataset at the given index.

Parameters

idx (int) – The index of the sample to retrieve.

Returns

A tuple consisting of:

- x (torch.Tensor): The head and relation part of the triple.
- y_idx (torch.Tensor): The concatenated indices of the true object (tail entity) and the indices of the negative samples.
- y_vec (torch.Tensor): A vector containing the labels for the positive and negative samples, with label smoothing applied.

Return type

tuple

class dicee.KvsSampleDataset (train_set_idx: numpy.ndarray, entity_idxs, relation_idxs, form, store=None, neg_ratio=None, label_smoothing_rate: float = 0.0)

Bases: torch.utils.data.Dataset

KvsSample a Dataset:

D:= {(x,y)_i}_i ^N, where

. x:(h,r) is a unique h in E and a relation r in R and . y in [0,1]^{|E|} is a binary label.

overall **y_i = 1** s.t. **(h r E_i)** in KG

At each mini-batch construction, we subsample(y), hence n

|new_y| << |E| new_y contains all 1's if sum(y) < neg_sample ratio new_y contains

train_set_idx

Indexed triples for the training.

entity_idxs

mapping.

```

relation_idxs
    mapping.

form
    ?

store
    ?

label_smoothing_rate
    ?

Bases: 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_set
length
num_entities
num_relations

```

```

__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.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.

`setup(*args, **kwargs)`

Called at the beginning of fit (train + validate), validate, test, or predict. This is a good hook when you need to build models dynamically or adjust something about them. This hook is called on every process when using DDP.

Parameters

- `stage` – either 'fit', 'validate', 'test', or 'predict'

Example:

```
class LitModel(...):
    def __init__(self):
        self.ll = None

    def prepare_data(self):
        download_data()
        tokenize()

        # don't do this
        self.something = else

    def setup(self, stage):
        data = load_data(...)
        self.ll = nn.Linear(28, data.num_classes)
```

`transfer_batch_to_device(*args, **kwargs)`

Override this hook if your `DataLoader` returns tensors wrapped in a custom data structure.

The data types listed below (and any arbitrary nesting of them) are supported out of the box:

- `torch.Tensor` or anything that implements `.to(...)`
- list
- dict
- tuple

For anything else, you need to define how the data is moved to the target device (CPU, GPU, TPU, ...).

Note

This hook should only transfer the data and not modify it, nor should it move the data to any other device than the one passed in as argument (unless you know what you are doing). To check the current state of execution of this hook you can use `self.trainer.training/testing/validating/predicting` so that you can add different logic as per your requirement.

Parameters

- `batch` – A batch of data that needs to be transferred to a new device.

- **device** – The target device as defined in PyTorch.
- **dataloader_idx** – The index of the dataloader to which the batch belongs.

Returns

A reference to the data on the new device.

Example:

```
def transfer_batch_to_device(self, batch, device, dataloader_idx):
    if isinstance(batch, CustomBatch):
        # move all tensors in your custom data structure to the device
        batch.samples = batch.samples.to(device)
        batch.targets = batch.targets.to(device)
    elif dataloader_idx == 0:
        # skip device transfer for the first dataloader or anything you wish
        # pass
    else:
        batch = super().transfer_batch_to_device(batch, device, dataloader_
→idx)
    return batch
```

See also

- `move_data_to_device()`
- `apply_to_collection()`

`prepare_data(*args, **kwargs)`

Use this to download and prepare data. Downloading and saving data with multiple processes (distributed settings) will result in corrupted data. Lightning ensures this method is called only within a single process, so you can safely add your downloading logic within.

⚠ Warning

DO NOT set state to the model (use `setup` instead) since this is NOT called on every device

Example:

```
def prepare_data(self):
    # good
    download_data()
    tokenize()
    etc()

    # bad
    self.split = data_split
    self.some_state = some_other_state()
```

In a distributed environment, `prepare_data` can be called in two ways (using `prepare_data_per_node`)

1. Once per node. This is the default and is only called on `LOCAL_RANK=0`.
2. Once in total. Only called on `GLOBAL_RANK=0`.

Example:

```
# DEFAULT
# called once per node on LOCAL_RANK=0 of that node
class LitDataModule(LightningDataModule):
    def __init__(self):
        super().__init__()
        self.prepare_data_per_node = True

# call on GLOBAL_RANK=0 (great for shared file systems)
class LitDataModule(LightningDataModule):
    def __init__(self):
        super().__init__()
        self.prepare_data_per_node = False
```

This is called before requesting the dataloaders:

```
model.prepare_data()
initialize_distributed()
model.setup(stage)
model.train_dataloader()
model.val_dataloader()
model.test_dataloader()
model.predict_dataloader()

class dicee.LiteralDataset(file_path: str, ent_idx: dict = None, normalization_type: str = 'z-norm',
                           sampling_ratio: float = None, loader_backend: str = 'pandas')
```

Bases: torch.utils.data.Dataset

Dataset for loading and processing literal data for training Literal Embedding model. This dataset handles the loading, normalization, and preparation of triples for training a literal embedding model.

Extends torch.utils.data.Dataset for supporting PyTorch dataloaders.

train_file_path

Path to the training data file.

Type

str

normalization

Type of normalization to apply ('z-norm', 'min-max', or None).

Type

str

normalization_params

Parameters used for normalization.

Type

dict

sampling_ratio

Fraction of the training set to use for ablations.

Type

float

```

entity_to_idx
    Mapping of entities to their indices.

    Type
        dict

num_entities
    Total number of entities.

    Type
        int

data_property_to_idx
    Mapping of data properties to their indices.

    Type
        dict

num_data_properties
    Total number of data properties.

    Type
        int

loader_backend
    Backend to use for loading data ('pandas' or 'rdflib').

    Type
        str

train_file_path
loader_backend = 'pandas'

normalization_type = 'z-norm'

normalization_params

sampling_ratio = None

entity_to_idx = None

num_entities

__getitem__(index)

__len__()

static load_and_validate_literal_data(file_path: str = None, loader_backend: str = 'pandas')
    → pandas.DataFrame

    Loads and validates the literal data file. :param file_path: Path to the literal data file. :type file_path: str

    Returns
        DataFrame containing the loaded and validated data.

    Return type
        pd.DataFrame

```

```

static denormalize(preds_norm, attributes, normalization_params) → numpy.ndarray
    Denormalizes the predictions based on the normalization type.

    Args: preds_norm (np.ndarray): Normalized predictions to be denormalized. attributes (list): List of attributes corresponding to the predictions. normalization_params (dict): Dictionary containing normalization parameters for each attribute.

    Returns
        Denormalized predictions.

    Return type
        np.ndarray

class dicee.QueryGenerator(train_path: str, test_path: str, ent2id: Dict = None, rel2id: Dict = None, seed: int = 1, gen_valid: bool = False, gen_test: bool = True)

    train_path
    val_path
    test_path
    gen_valid = False
    gen_test = True
    seed = 1
    max_ans_num = 1000000.0
    mode
    ent2id = None
    rel2id: Dict = None
    ent_in: Dict
    ent_out: Dict
    query_name_to_struct
    list2tuple(list_data)
    tuple2list(x: List | Tuple) → List | Tuple
        Convert a nested tuple to a nested list.

    set_global_seed(seed: int)
        Set seed

    construct_graph(paths: List[str]) → Tuple[Dict, Dict]
        Construct graph from triples Returns dicts with incoming and outgoing edges

    fill_query(query_structure: List[str | List], ent_in: Dict, ent_out: Dict, answer: int) → bool
        Private method for fill_query logic.

    achieve_answer(query: List[str | List], ent_in: Dict, ent_out: Dict) → set
        Private method for achieve_answer logic. @TODO: Document the code

    write_links(ent_out, small_ent_out)

```

```

ground_queries (query_structure: List[str | List], ent_in: Dict, ent_out: Dict, small_ent_in: Dict,
    small_ent_out: Dict, gen_num: int, query_name: str)
    Generating queries and achieving answers

unmap (query_type, queries, tp_answers, fp_answers, fn_answers)

unmap_query (query_structure, query, id2ent, id2rel)

generate_queries (query_struct: List, gen_num: int, query_type: str)
    Passing incoming and outgoing edges to ground queries depending on mode [train valid or text] and getting
    queries and answers in return @ TODO: create a class for each single query struct

save_queries (query_type: str, gen_num: int, save_path: str)

abstract load_queries (path)

get_queries (query_type: str, gen_num: int)

static save_queries_and_answers (path: str, data: List[Tuple[str, Tuple[collections.defaultdict]]])
    → None
    Save Queries into Disk

static load_queries_and_answers (path: str) → List[Tuple[str, Tuple[collections.defaultdict]]]
    Load Queries from Disk to Memory

dicee.__version__ = '0.1.5'

```

Python Module Index

d

dicee, 12
dicee.__main__, 12
dicee.abstracts, 12
dicee.analyse_experiments, 19
dicee.callbacks, 20
dicee.config, 29
dicee.dataset_classes, 32
dicee.eval_static_funcs, 46
dicee.evaluator, 48
dicee.executer, 49
dicee.knowledge_graph, 51
dicee.knowledge_graph_embeddings, 53
dicee.models, 56
dicee.models.adopt, 56
dicee.models.base_model, 58
dicee.models.clifford, 67
dicee.models.complex, 74
dicee.models.duale, 76
dicee.models.ensemble, 77
dicee.models.function_space, 78
dicee.models.literal, 82
dicee.models.octonion, 83
dicee.models.pykeen_models, 86
dicee.models.quaternion, 87
dicee.models.real, 90
dicee.models.static_funcs, 92
dicee.models.transformers, 92
dicee.query_generator, 146
dicee.read_preprocess_save_load_kg, 148
dicee.read_preprocess_save_load_kg.preprocess,
 148
dicee.read_preprocess_save_load_kg.read_from_disk,
 149
dicee.read_preprocess_save_load_kg.save_load_disk,
 149
dicee.read_preprocess_save_load_kg.util,
 150
dicee.sanity_checkers, 154
dicee.scripts, 155
dicee.scripts.index_serve, 155
dicee.scripts.run, 158
dicee.static_funcs, 158
dicee.static_funcs_training, 161
dicee.static_preprocess_funcs, 162
dicee.trainer, 163
dicee.trainer.dice_trainer, 163
dicee.trainer.model_parallelism, 165
dicee.trainer.torch_trainer, 165
dicee.trainer.torch_trainer_ddp, 167

Index

Non-alphabetical

`__call__()` (*dicee.EnsembleKGE method*), 196
`__call__()` (*dicee.models.base_model.IdentityClass method*), 67
`__call__()` (*dicee.models.ensemble.EnsembleKGE method*), 78
`__call__()` (*dicee.models.IdentityClass method*), 109, 121, 127
`__class_vars__` (*dicee.scripts.index_serve.StringListRequest attribute*), 156
`__getitem__()` (*dicee.AllvsAll method*), 208
`__getitem__()` (*dicee.BPE_NegativeSamplingDataset method*), 204
`__getitem__()` (*dicee.dataset_classes.AllvsAll method*), 37
`__getitem__()` (*dicee.dataset_classes.BPE_NegativeSamplingDataset method*), 34
`__getitem__()` (*dicee.dataset_classes.KvsAll method*), 36
`__getitem__()` (*dicee.dataset_classes.KvsSampleDataset method*), 39
`__getitem__()` (*dicee.dataset_classes.LiteralDataset method*), 45
`__getitem__()` (*dicee.dataset_classes.MultiClassClassificationDataset method*), 35
`__getitem__()` (*dicee.dataset_classes.MultiLabelDataset method*), 34
`__getitem__()` (*dicee.dataset_classes.NegSampleDataset method*), 40
`__getitem__()` (*dicee.dataset_classes.OnevsAllDataset method*), 35
`__getitem__()` (*dicee.dataset_classes.OnevsSample method*), 38
`__getitem__()` (*dicee.dataset_classes.TriplePredictionDataset method*), 41
`__getitem__()` (*dicee.KvsAll method*), 207
`__getitem__()` (*dicee.KvsSampleDataset method*), 210
`__getitem__()` (*dicee.LiteralDataset method*), 216
`__getitem__()` (*dicee.MultiClassClassificationDataset method*), 206
`__getitem__()` (*dicee.MultiLabelDataset method*), 205
`__getitem__()` (*dicee.NegSampleDataset method*), 211
`__getitem__()` (*dicee.OnevsAllDataset method*), 206
`__getitem__()` (*dicee.OnevsSample method*), 209
`__getitem__()` (*dicee.TriplePredictionDataset method*), 211
`__iter__()` (*dicee.config.Namespace method*), 32
`__iter__()` (*dicee.EnsembleKGE method*), 196
`__iter__()` (*dicee.knowledge_graph.KG method*), 52
`__iter__()` (*dicee.models.ensemble.EnsembleKGE method*), 78
`__len__()` (*dicee.AllvsAll method*), 208
`__len__()` (*dicee.BPE_NegativeSamplingDataset method*), 204
`__len__()` (*dicee.dataset_classes.AllvsAll method*), 37
`__len__()` (*dicee.dataset_classes.BPE_NegativeSamplingDataset method*), 34
`__len__()` (*dicee.dataset_classes.KvsAll method*), 36
`__len__()` (*dicee.dataset_classes.KvsSampleDataset method*), 39
`__len__()` (*dicee.dataset_classes.LiteralDataset method*), 46
`__len__()` (*dicee.dataset_classes.MultiClassClassificationDataset method*), 35
`__len__()` (*dicee.dataset_classes.MultiLabelDataset method*), 34
`__len__()` (*dicee.dataset_classes.NegSampleDataset method*), 40
`__len__()` (*dicee.dataset_classes.OnevsAllDataset method*), 35
`__len__()` (*dicee.dataset_classes.OnevsSample method*), 38
`__len__()` (*dicee.dataset_classes.TriplePredictionDataset method*), 41
`__len__()` (*dicee.EnsembleKGE method*), 196
`__len__()` (*dicee.knowledge_graph.KG method*), 52
`__len__()` (*dicee.KvsAll method*), 207
`__len__()` (*dicee.KvsSampleDataset method*), 210
`__len__()` (*dicee.LiteralDataset method*), 216
`__len__()` (*dicee.models.ensemble.EnsembleKGE method*), 78
`__len__()` (*dicee.MultiClassClassificationDataset method*), 206
`__len__()` (*dicee.MultiLabelDataset method*), 205
`__len__()` (*dicee.NegSampleDataset method*), 210
`__len__()` (*dicee.OnevsAllDataset method*), 206
`__len__()` (*dicee.OnevsSample method*), 209
`__len__()` (*dicee.TriplePredictionDataset method*), 211
`__private_attributes__` (*dicee.scripts.index_serve.StringListRequest attribute*), 157
`__pydantic_complete__` (*dicee.scripts.index_serve.StringListRequest attribute*), 157
`__pydantic_computed_fields__` (*dicee.scripts.index_serve.StringListRequest attribute*), 157
`__pydantic_core_schema__` (*dicee.scripts.index_serve.StringListRequest attribute*), 157
`__pydantic_custom_init__` (*dicee.scripts.index_serve.StringListRequest attribute*), 157
`__pydantic_decorators__` (*dicee.scripts.index_serve.StringListRequest attribute*), 157
`__pydantic_extra__` (*dicee.scripts.index_serve.StringListRequest attribute*), 157
`__pydantic_fields__` (*dicee.scripts.index_serve.StringListRequest attribute*), 157

```

__pydantic_fields_set__(dicee.scripts.index_serve.StringListRequest attribute), 157
__pydantic_generic_metadata__(dicee.scripts.index_serve.StringListRequest attribute), 157
__pydantic_parent_namespace__(dicee.scripts.index_serve.StringListRequest attribute), 157
__pydantic_post_init__(dicee.scripts.index_serve.StringListRequest attribute), 157
__pydantic_private__(dicee.scripts.index_serve.StringListRequest attribute), 157
__pydantic_root_model__(dicee.scripts.index_serve.StringListRequest attribute), 157
__pydantic_serializer__(dicee.scripts.index_serve.StringListRequest attribute), 157
__pydantic_validator__(dicee.scripts.index_serve.StringListRequest attribute), 157
__setstate__(dicee.models.ADOPT method), 100
__setstate__(dicee.models.adopt.ADOPT method), 57
__signature__(dicee.scripts.index_serve.StringListRequest attribute), 157
__str__(dicee.EnsembleKGE method), 196
__str__(dicee.KGE method), 199
__str__(dicee.knowledge_graph_embeddings.KGE method), 53
__str__(dicee.models.ensemble.EnsembleKGE method), 78
__version__(in module dicee), 218

```

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), 147
achieve_answer() (dicee.QueryGenerator method), 217
AConEx (class in dicee), 182
AConEx (class in dicee.models), 116
AConEx (class in dicee.models.complex), 75
AConvO (class in dicee), 182
AConvO (class in dicee.models), 129
AConvO (class in dicee.models.octonion), 85
AConvQ (class in dicee), 183
AConvQ (class in dicee.models), 123
AConvQ (class in dicee.models.quaternion), 90
adaptive_lr (dicee.config.Namespace attribute), 32
adaptive_swa (dicee.config.Namespace attribute), 32
add_new_entity_embeddings() (dicee.abstracts.BaseInteractiveKGE method), 15
add_noise_rate (dicee.config.Namespace attribute), 30
add_noise_rate (dicee.knowledge_graph.KG attribute), 51
add_noisy_triples() (in module dicee), 197
add_noisy_triples() (in module dicee.static_funcs), 160
add_noisy_triples_into_training() (dicee.read_preprocess_save_load_kg.read_from_disk.ReadFromDisk method), 149
add_noisy_triples_into_training() (dicee.read_preprocess_save_load_kg.ReadFromDisk method), 154
add_reciprocal (dicee.knowledge_graph.KG attribute), 52
ADOPT (class in dicee.models), 100
ADOPT (class in dicee.models.adopt), 57
adopt() (in module dicee.models.adopt), 57
AllvsAll (class in dicee), 207
AllvsAll (class in dicee.dataset_classes), 36
alphas (dicee.abstracts.AbstractPPECallback attribute), 18
alphas (dicee.callbacks.ASWA attribute), 24
analyse() (in module dicee.analyse_experiments), 20
answer_multi_hop_query() (dicee.KGE method), 201
answer_multi_hop_query() (dicee.knowledge_graph_embeddings.KGE method), 55
app (in module dicee.scripts.index_serve), 156
apply_coefficients() (dicee.DeCaL method), 178
apply_coefficients() (dicee.Keci method), 175
apply_coefficients() (dicee.models.clifford.DeCaL method), 72
apply_coefficients() (dicee.models.clifford.Keci method), 68
apply_coefficients() (dicee.models.DeCaL method), 135
apply_coefficients() (dicee.models.Keci method), 131
apply_reciprical_or_noise() (in module dicee.read_preprocess_save_load_kg.util), 152
apply_semantic_constraint (dicee.abstracts.BaseInteractiveKGE attribute), 14
apply_unit_norm (dicee.BaseKGE attribute), 194
apply_unit_norm (dicee.models.base_model.BaseKGE attribute), 64
apply_unit_norm (dicee.models.BaseKGE attribute), 107, 110, 114, 119, 125, 137, 141
args (dicee.BaseKGE attribute), 194
args (dicee.DICE_Trainer attribute), 198

```

```

args (dicee.evaluator.Evaluator attribute), 48
args (dicee.Execute attribute), 203
args (dicee.executor.Execute attribute), 49
args (dicee.models.base_model.BaseKGE attribute), 64
args (dicee.models.base_model.IdentityClass attribute), 66
args (dicee.models.BaseKGE attribute), 107, 110, 114, 118, 124, 137, 140
args (dicee.models.IdentityClass attribute), 109, 121, 127
args (dicee.models.pykeen_models.PykeenKGE attribute), 87
args (dicee.models.PykeenKGE attribute), 139
args (dicee.PykeenKGE attribute), 190
args (dicee.trainer.DICE_Trainer attribute), 168
args (dicee.trainer.dice_trainer.DICE_Trainer attribute), 163
ASWA (class in dicee.callbacks), 24
aswa (dicee.analyse_experiments.Experiment attribute), 19
attn (dicee.models.transformers.Block attribute), 97
attn_dropout (dicee.models.transformers.CausalSelfAttention attribute), 96
attributes (dicee.abtracts.AbstractTrainer attribute), 13
auto_batch_finding (dicee.config.Namespace attribute), 32

```

B

```

backend (dicee.config.Namespace attribute), 30
backend (dicee.knowledge_graph.KG attribute), 52
BaseInteractiveKGE (class in dicee.abtracts), 14
BaseInteractiveTrainKGE (class in dicee.abtracts), 18
BaseKGE (class in dicee), 193
BaseKGE (class in dicee.models), 106, 110, 113, 118, 124, 137, 140
BaseKGE (class in dicee.models.base_model), 63
BaseKGELightning (class in dicee.models), 101
BaseKGELightning (class in dicee.models.base_model), 58
batch_kronecker_product () (dicee.callbacks.KronE static method), 26
batch_size (dicee.analyse_experiments.Experiment attribute), 19
batch_size (dicee.callbacks.PseudoLabellingCallback attribute), 24
batch_size (dicee.config.Namespace attribute), 30
batch_size (dicee.CVDataModule attribute), 212
batch_size (dicee.dataset_classes.CVDataModule attribute), 41
batches_per_epoch (dicee.callbacks.LRScheduler attribute), 28
bias (dicee.models.transformers.GPTConfig attribute), 98
bias (dicee.models.transformers.LayerNorm attribute), 95
Block (class in dicee.models.transformers), 97
block_size (dicee.BaseKGE attribute), 195
block_size (dicee.config.Namespace attribute), 32
block_size (dicee.dataset_classes.MultiClassClassificationDataset attribute), 35
block_size (dicee.models.base_model.BaseKGE attribute), 65
block_size (dicee.models.BaseKGE attribute), 108, 111, 115, 119, 125, 138, 141
block_size (dicee.models.transformers.GPTConfig attribute), 97
block_size (dicee.MultiClassClassificationDataset attribute), 205
bn_conv1 (dicee.AConvQ attribute), 183
bn_conv1 (dicee.ConvQ attribute), 184
bn_conv1 (dicee.models.AConvQ attribute), 124
bn_conv1 (dicee.models.ConvQ attribute), 123
bn_conv1 (dicee.models.quaternion.AConvQ attribute), 90
bn_conv1 (dicee.models.quaternion.ConvQ attribute), 89
bn_conv2 (dicee.AConvQ attribute), 183
bn_conv2 (dicee.ConvQ attribute), 184
bn_conv2 (dicee.models.AConvQ attribute), 124
bn_conv2 (dicee.models.ConvQ attribute), 123
bn_conv2 (dicee.models.quaternion.AConvQ attribute), 90
bn_conv2 (dicee.models.quaternion.ConvQ attribute), 89
bn_conv2d (dicee.AConEx attribute), 182
bn_conv2d (dicee.AConvO attribute), 183
bn_conv2d (dicee.ConEx attribute), 186
bn_conv2d (dicee.ConvO attribute), 185
bn_conv2d (dicee.models.AConEx attribute), 116
bn_conv2d (dicee.models.AConvO attribute), 129
bn_conv2d (dicee.models.complex.AConEx attribute), 75
bn_conv2d (dicee.models.complex.ConEx attribute), 74
bn_conv2d (dicee.models.ConEx attribute), 116

```

bn_conv2d (*dicee.models.ConvO attribute*), 129
 bn_conv2d (*dicee.models.octonion.AConvO attribute*), 86
 bn_conv2d (*dicee.models.octonion.ConvO attribute*), 85
 BPE_NegativeSamplingDataset (*class in dicee*), 204
 BPE_NegativeSamplingDataset (*class in dicee.dataset_classes*), 33
 build_chain_funcs () (*dicee.models.FMult2 method*), 144
 build_chain_funcs () (*dicee.models.function_space.FMult2 method*), 80
 build_func () (*dicee.models.FMult2 method*), 144
 build_func () (*dicee.models.function_space.FMult2 method*), 80
 Byte (*class in dicee*), 191
 Byte (*class in dicee.models.transformers*), 93
 byte_pair_encoding (*dicee.analyse_experiments.Experiment attribute*), 19
 byte_pair_encoding (*dicee.BaseKGE attribute*), 194
 byte_pair_encoding (*dicee.config.Namespace attribute*), 32
 byte_pair_encoding (*dicee.knowledge_graph.KG attribute*), 51
 byte_pair_encoding (*dicee.models.base_model.BaseKGE attribute*), 65
 byte_pair_encoding (*dicee.models.BaseKGE attribute*), 108, 111, 115, 119, 125, 138, 141

C

c_attn (*dicee.models.transformers.CausalSelfAttention attribute*), 95
 c_fc (*dicee.models.transformers.MLP attribute*), 96
 c_proj (*dicee.models.transformers.CausalSelfAttention attribute*), 96
 c_proj (*dicee.models.transformers.MLP attribute*), 96
 callbacks (*dicee.abstracts.AbstractTrainer attribute*), 13
 callbacks (*dicee.analyse_experiments.Experiment attribute*), 19
 callbacks (*dicee.config.Namespace attribute*), 30
 callbacks (*dicee.trainer.torch_trainer_ddp.NodeTrainer attribute*), 168
 CausalSelfAttention (*class in dicee.models.transformers*), 95
 chain_func () (*dicee.models.FMult method*), 143
 chain_func () (*dicee.models.function_space.FMult method*), 79
 chain_func () (*dicee.models.function_space.GFMult method*), 79
 chain_func () (*dicee.models.GFMult method*), 143
 CKeci (*class in dicee*), 173
 CKeci (*class in dicee.models*), 133
 CKeci (*class in dicee.models.clifford*), 70
 cl_pqr () (*dicee.DeCaL method*), 177
 cl_pqr () (*dicee.models.clifford.DeCaL method*), 71
 cl_pqr () (*dicee.models.DeCaL method*), 134
 clifford_multiplication () (*dicee.Keci method*), 175
 clifford_multiplication () (*dicee.models.clifford.Keci method*), 68
 clifford_multiplication () (*dicee.models.Keci method*), 131
 clip_lambda (*dicee.models.ADOPT attribute*), 100
 clip_lambda (*dicee.models.adopt.ADOPT attribute*), 57
 collate_fn (*dicee.AllvsAll attribute*), 208
 collate_fn (*dicee.dataset_classes.AllvsAll attribute*), 37
 collate_fn (*dicee.dataset_classes.KvsAll attribute*), 36
 collate_fn (*dicee.dataset_classes.KvsSampleDataset attribute*), 39
 collate_fn (*dicee.dataset_classes.MultiClassClassificationDataset attribute*), 35
 collate_fn (*dicee.dataset_classes.MultiLabelDataset attribute*), 34
 collate_fn (*dicee.dataset_classes.OnevsAllDataset attribute*), 35
 collate_fn (*dicee.dataset_classes.OnevsSample attribute*), 38
 collate_fn (*dicee.KvsAll attribute*), 207
 collate_fn (*dicee.KvsSampleDataset attribute*), 210
 collate_fn (*dicee.MultiClassClassificationDataset attribute*), 206
 collate_fn (*dicee.MultiLabelDataset attribute*), 205
 collate_fn (*dicee.OnevsAllDataset attribute*), 206
 collate_fn (*dicee.OnevsSample attribute*), 208, 209
 collate_fn () (*dicee.BPE_NegativeSamplingDataset method*), 205
 collate_fn () (*dicee.dataset_classes.BPE_NegativeSamplingDataset method*), 34
 collate_fn () (*dicee.dataset_classes.TriplePredictionDataset method*), 41
 collate_fn () (*dicee.TriplePredictionDataset method*), 211
 collection_name (*dicee.scripts.index_serve.NeuralSearcher attribute*), 156
 comp_func () (*dicee.LFMult method*), 190
 comp_func () (*dicee.models.function_space.LFMult method*), 81
 comp_func () (*dicee.models.LFMult method*), 145
 ComplEx (*class in dicee*), 181
 ComplEx (*class in dicee.models*), 117

ComplEx (*class in dicee.models.complex*), 75
 compute_convergence() (*in module dicee.callbacks*), 24
 compute_func() (*dicee.models.FMult method*), 143
 compute_func() (*dicee.models.FMult2 method*), 144
 compute_func() (*dicee.models.function_space.FMult method*), 79
 compute_func() (*dicee.models.function_space.FMult2 method*), 80
 compute_func() (*dicee.models.function_space.GFMult method*), 79
 compute_func() (*dicee.models.GFMult method*), 143
 compute_mrr() (*dicee.callbacks.ASWA static method*), 25
 compute_sigma_pp() (*dicee.DeCaL method*), 178
 compute_sigma_pp() (*dicee.Keci method*), 174
 compute_sigma_pp() (*dicee.models.clifford.DeCaL method*), 72
 compute_sigma_pp() (*dicee.models.clifford.Keci method*), 68
 compute_sigma_pp() (*dicee.models.DeCaL method*), 135
 compute_sigma_pp() (*dicee.models.Keci method*), 131
 compute_sigma_pq() (*dicee.DeCaL method*), 179
 compute_sigma_pq() (*dicee.Keci method*), 174
 compute_sigma_pq() (*dicee.models.clifford.DeCaL method*), 73
 compute_sigma_pq() (*dicee.models.clifford.Keci method*), 68
 compute_sigma_pq() (*dicee.models.DeCaL method*), 136
 compute_sigma_pq() (*dicee.models.Keci method*), 131
 compute_sigma_pr() (*dicee.DeCaL method*), 180
 compute_sigma_pr() (*dicee.models.clifford.DeCaL method*), 73
 compute_sigma_pr() (*dicee.models.DeCaL method*), 136
 compute_sigma_qq() (*dicee.DeCaL method*), 179
 compute_sigma_qq() (*dicee.Keci method*), 174
 compute_sigma_qq() (*dicee.models.clifford.DeCaL method*), 73
 compute_sigma_qq() (*dicee.models.clifford.Keci method*), 68
 compute_sigma_qq() (*dicee.models.DeCaL method*), 135
 compute_sigma_qq() (*dicee.models.Keci method*), 131
 compute_sigma_qr() (*dicee.DeCaL method*), 180
 compute_sigma_qr() (*dicee.models.clifford.DeCaL method*), 74
 compute_sigma_qr() (*dicee.models.DeCaL method*), 136
 compute_sigma_rr() (*dicee.DeCaL method*), 179
 compute_sigma_rr() (*dicee.models.clifford.DeCaL method*), 73
 compute_sigma_rr() (*dicee.models.DeCaL method*), 136
 compute_sigmas_multivect() (*dicee.DeCaL method*), 178
 compute_sigmas_multivect() (*dicee.models.clifford.DeCaL method*), 71
 compute_sigmas_multivect() (*dicee.models.DeCaL method*), 134
 compute_sigmas_single() (*dicee.DeCaL method*), 177
 compute_sigmas_single() (*dicee.models.clifford.DeCaL method*), 71
 compute_sigmas_single() (*dicee.models.DeCaL method*), 134
 ConeEx (*class in dicee*), 185
 ConeEx (*class in dicee.models*), 116
 ConeEx (*class in dicee.models.complex*), 74
 config (*dicee.BytE attribute*), 192
 config (*dicee.models.transformers.BytE attribute*), 93
 config (*dicee.models.transformers.GPT attribute*), 98
 configs (*dicee.abstracts.BaseInteractiveKGE attribute*), 14
 configure_optimizers() (*dicee.models.base_model.BaseKGELightning method*), 62
 configure_optimizers() (*dicee.models.BaseKGELightning method*), 105
 configure_optimizers() (*dicee.models.transformers.GPT method*), 99
 construct_batch_selected_cl_multivector() (*dicee.Keci method*), 175
 construct_batch_selected_cl_multivector() (*dicee.models.clifford.Keci method*), 69
 construct_batch_selected_cl_multivector() (*dicee.models.Keci method*), 132
 construct_cl_multivector() (*dicee.DeCaL method*), 178
 construct_cl_multivector() (*dicee.Keci method*), 175
 construct_cl_multivector() (*dicee.models.clifford.DeCaL method*), 72
 construct_cl_multivector() (*dicee.models.clifford.Keci method*), 69
 construct_cl_multivector() (*dicee.models.DeCaL method*), 135
 construct_cl_multivector() (*dicee.models.Keci method*), 132
 construct_dataset() (*in module dicee*), 204
 construct_dataset() (*in module dicee.dataset_classes*), 33
 construct_ensemble (*dicee.abstracts.BaseInteractiveKGE attribute*), 14
 construct_graph() (*dicee.query_generator.QueryGenerator method*), 147
 construct_graph() (*dicee.QueryGenerator method*), 217
 construct_input_and_output() (*dicee.abstracts.BaseInteractiveKGE method*), 16
 construct_multi_coeff() (*dicee.LFMult method*), 189

construct_multi_coeff () (*dicee.models.function_space.LFMult method*), 81
 construct_multi_coeff () (*dicee.models.LFMult method*), 145
 continual_learning (*dicee.config.Namespace attribute*), 32
 continual_start () (*dicee.DICE_Trainer method*), 198
 continual_start () (*dicee.executer.ContinuousExecute method*), 51
 continual_start () (*dicee.trainer.DICE_Trainer method*), 168
 continual_start () (*dicee.trainer.dice_trainer.DICE_Trainer method*), 164
 continual_training_setup_executor () (*in module dicee*), 197
 continual_training_setup_executor () (*in module dicee.static_funcs*), 161
 ContinuousExecute (*class in dicee.executer*), 50
 conv2d (*dicee.AConEx attribute*), 182
 conv2d (*dicee.AConvO attribute*), 183
 conv2d (*dicee.AConvQ attribute*), 183
 conv2d (*dicee.ConEx attribute*), 185
 conv2d (*dicee.ConvO attribute*), 185
 conv2d (*dicee.ConvQ attribute*), 184
 conv2d (*dicee.models.AConEx attribute*), 116
 conv2d (*dicee.models.AConvO attribute*), 129
 conv2d (*dicee.models.AConvQ attribute*), 123
 conv2d (*dicee.models.complex.AConEx attribute*), 75
 conv2d (*dicee.models.complex.ConEx attribute*), 74
 conv2d (*dicee.models.ConEx attribute*), 116
 conv2d (*dicee.models.ConvO attribute*), 129
 conv2d (*dicee.models.ConvQ attribute*), 123
 conv2d (*dicee.models.octonion.AConvO attribute*), 86
 conv2d (*dicee.models.octonion.ConvO attribute*), 85
 conv2d (*dicee.models.quaternion.AConvQ attribute*), 90
 conv2d (*dicee.models.quaternion.ConvQ attribute*), 89
 ConvO (*class in dicee*), 184
 ConvO (*class in dicee.models*), 128
 ConvO (*class in dicee.models.octonion*), 84
 ConvQ (*class in dicee*), 184
 ConvQ (*class in dicee.models*), 123
 ConvQ (*class in dicee.models.quaternion*), 89
 create_constraints () (*in module dicee.read_preprocess_save_load_kg.util*), 152
 create_constraints () (*in module dicee.static_funcs*), 162
 create_experiment_folder () (*in module dicee*), 197
 create_experiment_folder () (*in module dicee.static_funcs*), 161
 create_random_data () (*dicee.callbacks.PseudoLabellingCallback method*), 24
 create_reciprocal_triples () (*in module dicee*), 196
 create_reciprocal_triples () (*in module dicee.read_preprocess_save_load_kg.util*), 153
 create_reciprocal_triples () (*in module dicee.static_funcs*), 159
 create_vector_database () (*dicee.KGE method*), 199
 create_vector_database () (*dicee.knowledge_graph_embeddings.KGE method*), 53
 crop_block_size () (*dicee.models.transformers.GPT method*), 99
 ctx (*dicee.trainer.torch_trainer_ddp.NodeTrainer attribute*), 168
 current_epoch (*dicee.callbacks.SWA attribute*), 29
 CVDataModule (*class in dicee*), 211
 CVDataModule (*class in dicee.dataset_classes*), 41
 cycle_length (*dicee.callbacks.LRScheduler attribute*), 28

D

data_module (*dicee.callbacks.PseudoLabellingCallback attribute*), 24
 data_property_embeddings (*dicee.models.literal.LiteralEmbeddings attribute*), 83
 data_property_to_idx (*dicee.dataset_classes.LiteralDataset attribute*), 45
 data_property_to_idx (*dicee.literal_dataset attribute*), 216
 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*), 153
 DeCaL (*class in dicee*), 176
 DeCaL (*class in dicee.models*), 133
 DeCaL (*class in dicee.models.clifford*), 70
 decide () (*dicee.callbacks.ASWA method*), 25
 default_eval_model (*dicee.callbacks.PeriodicEvalCallback attribute*), 28
 degree (*dicee.LFMult attribute*), 189
 degree (*dicee.models.function_space.LFMult attribute*), 80
 degree (*dicee.models.LFMult attribute*), 144

```
denormalize() (dicee.dataset_classes.LiteralDataset static method), 46
denormalize() (dicee.LiteralDataset static method), 216
deploy() (dicee.KGE method), 202
deploy() (dicee.knowledge_graph_embeddings.KGE method), 56
deploy_head_entity_prediction() (in module dicee), 197
deploy_head_entity_prediction() (in module dicee.static_funcs), 160
deploy_relation_prediction() (in module dicee), 197
deploy_relation_prediction() (in module dicee.static_funcs), 161
deploy_tail_entity_prediction() (in module dicee), 197
deploy_tail_entity_prediction() (in module dicee.static_funcs), 160
deploy_triple_prediction() (in module dicee), 197
deploy_triple_prediction() (in module dicee.static_funcs), 160
describe() (dicee.knowledge_graph.KG method), 52
description_of_input (dicee.knowledge_graph.KG attribute), 52
device (dicee.models.literal.LiteralEmbeddings property), 83
DICE_Trainer (class in dicee), 198
DICE_Trainer (class in dicee.trainer), 168
DICE_Trainer (class in dicee.trainer.dice_trainer), 163
dicee
    module, 12
dicee.__main__
    module, 12
dicee.abstracts
    module, 12
dicee.analyse_experiments
    module, 19
dicee.callbacks
    module, 20
dicee.config
    module, 29
dicee.dataset_classes
    module, 32
dicee.eval_static_funcs
    module, 46
dicee.evaluator
    module, 48
dicee.executor
    module, 49
dicee.knowledge_graph
    module, 51
dicee.knowledge_graph_embeddings
    module, 53
dicee.models
    module, 56
dicee.models.adopt
    module, 56
dicee.models.base_model
    module, 58
dicee.models.clifford
    module, 67
dicee.models.complex
    module, 74
dicee.models.duale
    module, 76
dicee.models.ensemble
    module, 77
dicee.models.function_space
    module, 78
dicee.models.literal
    module, 82
dicee.models.octonion
    module, 83
dicee.models.pykeen_models
    module, 86
dicee.models.quaternion
    module, 87
dicee.models.real
    module, 90
```

```

dicee.models.static_funcs
    module, 92
dicee.models.transformers
    module, 92
dicee.query_generator
    module, 146
dicee.read_preprocess_save_load_kg
    module, 148
dicee.read_preprocess_save_load_kg.preprocess
    module, 148
dicee.read_preprocess_save_load_kg.read_from_disk
    module, 149
dicee.read_preprocess_save_load_kg.save_load_disk
    module, 149
dicee.read_preprocess_save_load_kg.util
    module, 150
dicee.sanity_checkers
    module, 154
dicee.scripts
    module, 155
dicee.scripts.index_serve
    module, 155
dicee.scripts.run
    module, 158
dicee.static_funcs
    module, 158
dicee.static_funcs_training
    module, 161
dicee.static_preprocess_funcs
    module, 162
dicee.trainer
    module, 163
dicee.trainer.dice_trainer
    module, 163
dicee.trainer.model_parallelism
    module, 165
dicee.trainer.torch_trainer
    module, 165
dicee.trainer.torch_trainer_ddp
    module, 167
discrete_points (dicee.models.FMult2 attribute), 143
discrete_points (dicee.models.function_space.FMult2 attribute), 80
dist_func (dicee.models.Pyke attribute), 113
dist_func (dicee.models.real.Pyke attribute), 92
dist_func (dicee.Pyke attribute), 172
DistMult (class in dicee), 172
DistMult (class in dicee.models), 112
DistMult (class in dicee.models.real), 91
download_file () (in module dicee), 197
download_file () (in module dicee.static_funcs), 161
download_files_from_url () (in module dicee), 197
download_files_from_url () (in module dicee.static_funcs), 161
download_pretrained_model () (in module dicee), 197
download_pretrained_model () (in module dicee.static_funcs), 161
dropout (dicee.models.literal.LiteralEmbeddings attribute), 82, 83
dropout (dicee.models.transformers.CausalSelfAttention attribute), 96
dropout (dicee.models.transformers.GPTConfig attribute), 98
dropout (dicee.models.transformers.MLP attribute), 97
DualE (class in dicee), 180
DualE (class in dicee.models), 145
DualE (class in dicee.models.dualE), 76
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), 162
 embedding_dim (dicee.analyse_experiments.Experiment attribute), 19
 embedding_dim (dicee.BaseKGE attribute), 194
 embedding_dim (dicee.config.Namespace attribute), 30
 embedding_dim (dicee.models.base_model.BaseKGE attribute), 64
 embedding_dim (dicee.models.BaseKGE attribute), 107, 110, 114, 118, 125, 137, 141
 embedding_dim (dicee.models.literal.LiteralEmbeddings attribute), 82
 embedding_dims (dicee.models.literal.LiteralEmbeddings attribute), 82
 enable_log (in module dicee.static_preprocess_funcs), 162
 enc (dicee.knowledge_graph.KG attribute), 52
 end() (dicee.Execute method), 203
 end() (dicee.executor.Execute method), 50
 EnsembleKGE (class in dicee), 195
 EnsembleKGE (class in dicee.models.ensemble), 78
 ent2id (dicee.query_generator.QueryGenerator attribute), 147
 ent2id (dicee.QueryGenerator attribute), 217
 ent_in (dicee.query_generator.QueryGenerator attribute), 147
 ent_in (dicee.QueryGenerator attribute), 217
 ent_out (dicee.query_generator.QueryGenerator attribute), 147
 ent_out (dicee.QueryGenerator attribute), 217
 entities_str (dicee.knowledge_graph.KG property), 52
 entity_embeddings (dicee.AConvQ attribute), 183
 entity_embeddings (dicee.ConvQ attribute), 184
 entity_embeddings (dicee.DeCaL attribute), 177
 entity_embeddings (dicee.DualE attribute), 180
 entity_embeddings (dicee.LFMult attribute), 189
 entity_embeddings (dicee.models.AConvQ attribute), 123
 entity_embeddings (dicee.models.clifford.DeCaL attribute), 71
 entity_embeddings (dicee.models.ConvQ attribute), 123
 entity_embeddings (dicee.models.DeCaL attribute), 134
 entity_embeddings (dicee.models.DualE attribute), 146
 entity_embeddings (dicee.models.dualE.DualE attribute), 76
 entity_embeddings (dicee.models.FMult attribute), 142
 entity_embeddings (dicee.models.FMult2 attribute), 143
 entity_embeddings (dicee.models.function_space.FMult attribute), 78
 entity_embeddings (dicee.models.function_space.FMult2 attribute), 80
 entity_embeddings (dicee.models.function_space.GFMult attribute), 79
 entity_embeddings (dicee.models.function_space.LFMult attribute), 80
 entity_embeddings (dicee.models.function_space.LFMult1 attribute), 80
 entity_embeddings (dicee.models.GFMult attribute), 143
 entity_embeddings (dicee.models.LFMult attribute), 144
 entity_embeddings (dicee.models.LFMult1 attribute), 144
 entity_embeddings (dicee.models.literal.LiteralEmbeddings attribute), 82, 83
 entity_embeddings (dicee.models.pykeen_models.PykeenKGE attribute), 87
 entity_embeddings (dicee.models.PykeenKGE attribute), 139
 entity_embeddings (dicee.models.quaternion.AConvQ attribute), 90
 entity_embeddings (dicee.models.quaternion.ConvQ attribute), 89
 entity_embeddings (dicee.PykeenKGE attribute), 190
 entity_to_idx (dicee.dataset_classes.LiteralDataset attribute), 45
 entity_to_idx (dicee.knowledge_graph.KG attribute), 52
 entity_to_idx (dicee.LiteralDataset attribute), 215, 216
 entity_to_idx (dicee.scripts.index_serve.NeuralSearcher attribute), 156
 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), 99
 estimate_q() (in module dicee.callbacks), 24
 Eval (class in dicee.callbacks), 25
 eval() (dicee.EnsembleKGE method), 196
 eval() (dicee.evaluator.Evaluator method), 48
 eval() (dicee.models.ensemble.EnsembleKGE method), 78
 eval_at_epochs (dicee.config.Namespace attribute), 32
 eval_epochs (dicee.callbacks.PeriodicEvalCallback attribute), 28
 eval_every_n_epochs (dicee.config.Namespace attribute), 32

eval_lp_performance() (*dicee.KGE method*), 199
 eval_lp_performance() (*dicee.knowledge_graph_embeddings.KGE method*), 53
 eval_model (*dicee.config.Namespace attribute*), 31
 eval_model (*dicee.knowledge_graph.KG attribute*), 52
 eval_rank_of_head_and_tail_byte_pair_encoded_entity() (*dicee.evaluator.Evaluator method*), 48
 eval_rank_of_head_and_tail_entity() (*dicee.evaluator.Evaluator method*), 48
 eval_with_bpe_vs_all() (*dicee.evaluator.Evaluator method*), 49
 eval_with_byte() (*dicee.evaluator.Evaluator method*), 49
 eval_with_data() (*dicee.evaluator.Evaluator method*), 49
 eval_with_vs_all() (*dicee.evaluator.Evaluator method*), 49
 evaluate() (*in module dicee*), 197
 evaluate() (*in module dicee.static_funcs*), 161
 evaluate_bpe_lp() (*in module dicee.static_funcs_training*), 162
 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*), 47
 evaluate_link_prediction_performance_with_reciprocals() (*in module dicee.eval_static_funcs*), 47
 evaluate_link_prediction_performance_with_reciprocals() (*in module dicee.eval_static_funcs*), 47
 evaluate_literal_prediction() (*in module dicee.eval_static_funcs*), 47
 evaluate_lp() (*dicee.evaluator.Evaluator method*), 49
 evaluate_lp() (*in module dicee.static_funcs_training*), 161
 evaluate_lp_bpe_k_vs_all() (*dicee.evaluator.Evaluator method*), 49
 evaluate_lp_bpe_k_vs_all() (*in module dicee.eval_static_funcs*), 47
 evaluate_lp_k_vs_all() (*dicee.evaluator.Evaluator method*), 49
 evaluate_lp_with_byte() (*dicee.evaluator.Evaluator method*), 49
 Executor (*class in dicee.evaluator*), 48
 evaluator (*dicee.DICE_Trainer attribute*), 198
 evaluator (*dicee.Execute attribute*), 203
 evaluator (*dicee.executer.Execute attribute*), 50
 evaluator (*dicee.trainer.DICE_Trainer attribute*), 168
 evaluator (*dicee.trainer.dice_trainer.DICE_Trainer attribute*), 164
 every_x_epoch (*dicee.callbacks.KGESaveCallback attribute*), 23
 example_input_array (*dicee.EnsembleKGE property*), 196
 example_input_array (*dicee.models.ensemble.EnsembleKGE property*), 78
 Execute (*class in dicee*), 203
 Execute (*class in dicee.executor*), 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*), 122
 explicit (*dicee.models.quaternion.QMult attribute*), 88
 explicit (*dicee.QMult attribute*), 187
 exponential_function() (*in module dicee*), 197
 exponential_function() (*in module dicee.static_funcs*), 161
 extract_input_outputs() (*dicee.trainer.torch_trainer_ddp.NodeTrainer method*), 168
 extract_input_outputs() (*in module dicee.trainer.model_parallelism*), 165
 extract_input_outputs_set_device() (*dicee.trainer.torch_trainer.TorchTrainer method*), 166

F

f (*dicee.callbacks.KronE attribute*), 26
 fc (*dicee.models.literal.LiteralEmbeddings attribute*), 83
 fc1 (*dicee.AConEx attribute*), 182
 fc1 (*dicee.AConvO attribute*), 183
 fc1 (*dicee.AConvQ attribute*), 183
 fc1 (*dicee.ConEx attribute*), 185
 fc1 (*dicee.ConvO attribute*), 185
 fc1 (*dicee.ConvQ attribute*), 184
 fc1 (*dicee.models.AConEx attribute*), 116
 fc1 (*dicee.models.AConvO attribute*), 129
 fc1 (*dicee.models.AConvQ attribute*), 124
 fc1 (*dicee.models.complex.AConEx attribute*), 75
 fc1 (*dicee.models.complex.ConEx attribute*), 74
 fc1 (*dicee.models.ConEx attribute*), 116
 fc1 (*dicee.models.ConvO attribute*), 129
 fc1 (*dicee.models.ConvQ attribute*), 123
 fc1 (*dicee.models.octonion.AConvO attribute*), 86

fc1 (*dicee.models.octonion.ConvO attribute*), 85
 fc1 (*dicee.models.quaternion.AConvQ attribute*), 90
 fc1 (*dicee.models.quaternion.ConvQ attribute*), 89
 fc_num_input (*dicee.AConEx attribute*), 182
 fc_num_input (*dicee.AConvO attribute*), 183
 fc_num_input (*dicee.AConvQ attribute*), 183
 fc_num_input (*dicee.ConEx attribute*), 185
 fc_num_input (*dicee.ConvO attribute*), 185
 fc_num_input (*dicee.ConvQ attribute*), 184
 fc_num_input (*dicee.models.AConEx attribute*), 116
 fc_num_input (*dicee.models.AConvO attribute*), 129
 fc_num_input (*dicee.models.AConvQ attribute*), 123
 fc_num_input (*dicee.models.complex.AConEx attribute*), 75
 fc_num_input (*dicee.models.complex.ConEx attribute*), 74
 fc_num_input (*dicee.models.ConEx attribute*), 116
 fc_num_input (*dicee.models.ConvO attribute*), 129
 fc_num_input (*dicee.models.ConvQ attribute*), 123
 fc_num_input (*dicee.models.octonion.AConvO attribute*), 86
 fc_num_input (*dicee.models.octonion.ConvO attribute*), 85
 fc_num_input (*dicee.models.quaternion.AConvQ attribute*), 90
 fc_num_input (*dicee.models.quaternion.ConvQ attribute*), 89
 fc_out (*dicee.models.literal.LiteralEmbeddings attribute*), 83
 feature_map_dropout (*dicee.AConEx attribute*), 182
 feature_map_dropout (*dicee.AConvO attribute*), 183
 feature_map_dropout (*dicee.AConvQ attribute*), 183
 feature_map_dropout (*dicee.ConEx attribute*), 186
 feature_map_dropout (*dicee.ConvO attribute*), 185
 feature_map_dropout (*dicee.ConvQ attribute*), 184
 feature_map_dropout (*dicee.models.AConEx attribute*), 116
 feature_map_dropout (*dicee.models.AConvO attribute*), 129
 feature_map_dropout (*dicee.models.AConvQ attribute*), 124
 feature_map_dropout (*dicee.models.complex.AConEx attribute*), 75
 feature_map_dropout (*dicee.models.complex.ConEx attribute*), 74
 feature_map_dropout (*dicee.models.ConEx attribute*), 116
 feature_map_dropout (*dicee.models.ConvO attribute*), 129
 feature_map_dropout (*dicee.models.ConvQ attribute*), 123
 feature_map_dropout (*dicee.models.octonion.AConvO attribute*), 86
 feature_map_dropout (*dicee.models.octonion.ConvO attribute*), 85
 feature_map_dropout (*dicee.models.quaternion.AConvQ attribute*), 90
 feature_map_dropout (*dicee.models.quaternion.ConvQ attribute*), 89
 feature_map_dropout_rate (*dicee.BaseKGE attribute*), 194
 feature_map_dropout_rate (*dicee.config.Namespace attribute*), 31
 feature_map_dropout_rate (*dicee.models.base_model.BaseKGE attribute*), 64
 feature_map_dropout_rate (*dicee.models.BaseKGE attribute*), 107, 110, 114, 119, 125, 138, 141
 fill_query () (*dicee.query_generator.QueryGenerator method*), 147
 fill_query () (*dicee.QueryGenerator method*), 217
 find_good_batch_size () (*in module dicee.trainer.model_parallelism*), 165
 find_missing_triples () (*dicee.KGE method*), 202
 find_missing_triples () (*dicee.knowledge_graph_embeddings.KGE method*), 55
 fit () (*dicee.trainer.model_parallelism.TensorParallel method*), 165
 fit () (*dicee.trainer.torch_trainer_ddp.TorchDDPTrainer method*), 167
 fit () (*dicee.trainer.torch.Trainer method*), 166
 flash (*dicee.models.transformers.CausalSelfAttention attribute*), 96
 FMult (*class in dicee.models*), 142
 FMult (*class in dicee.models.function_space*), 78
 FMult2 (*class in dicee.models*), 143
 FMult2 (*class in dicee.models.function_space*), 79
 form_of_labelling (*dicee.DICE_Trainer attribute*), 198
 form_of_labelling (*dicee.trainer.DICE_Trainer attribute*), 168
 form_of_labelling (*dicee.trainer.dice_trainer.DICE_Trainer attribute*), 164
 forward () (*dicee.BaseKGE method*), 195
 forward () (*dicee.BytE method*), 192
 forward () (*dicee.models.base_model.BaseKGE method*), 65
 forward () (*dicee.models.base_model.IdentityClass static method*), 67
 forward () (*dicee.models.BaseKGE method*), 108, 111, 115, 120, 126, 138, 142
 forward () (*dicee.models.IdentityClass static method*), 109, 121, 127
 forward () (*dicee.models.literal.LiteralEmbeddings method*), 83
 forward () (*dicee.models.transformers.Block method*), 97

```

forward() (dicee.models.transformers.BytE method), 93
forward() (dicee.models.transformers.CausalSelfAttention method), 96
forward() (dicee.models.transformers.GPT method), 98
forward() (dicee.models.transformers.LayerNorm method), 95
forward() (dicee.models.transformers.MLP method), 97
forward_backward_update() (dicee.trainer.torch_trainer.TorchTrainer method), 166
forward_backward_update_loss() (in module dicee.trainer.model_parallelism), 165
forward_byte_pair_encoded_k_vs_all() (dicee.BaseKGE method), 195
forward_byte_pair_encoded_k_vs_all() (dicee.models.base_model.BaseKGE method), 65
forward_byte_pair_encoded_k_vs_all() (dicee.models.BaseKGE method), 108, 111, 115, 119, 125, 138, 141
forward_byte_pair_encoded_triple() (dicee.BaseKGE method), 195
forward_byte_pair_encoded_triple() (dicee.models.base_model.BaseKGE method), 65
forward_byte_pair_encoded_triple() (dicee.models.BaseKGE method), 108, 111, 115, 119, 125, 138, 141
forward_k_vs_all() (dicee.AConEx method), 182
forward_k_vs_all() (dicee.ACovO method), 183
forward_k_vs_all() (dicee.AConvQ method), 183
forward_k_vs_all() (dicee.BaseKGE method), 195
forward_k_vs_all() (dicee.ComplEx method), 182
forward_k_vs_all() (dicee.ConEx method), 186
forward_k_vs_all() (dicee.ConvO method), 185
forward_k_vs_all() (dicee.ConvQ method), 184
forward_k_vs_all() (dicee.DeCaL method), 178
forward_k_vs_all() (dicee.DistMult method), 173
forward_k_vs_all() (dicee.DualE method), 181
forward_k_vs_all() (dicee.Keci method), 175
forward_k_vs_all() (dicee.models.AConEx method), 117
forward_k_vs_all() (dicee.models.ACovO method), 130
forward_k_vs_all() (dicee.models.AConvQ method), 124
forward_k_vs_all() (dicee.models.base_model.BaseKGE method), 65
forward_k_vs_all() (dicee.models.BaseKGE method), 108, 112, 115, 120, 126, 139, 142
forward_k_vs_all() (dicee.models.clifford.DeCaL method), 72
forward_k_vs_all() (dicee.models.clifford.Keci method), 69
forward_k_vs_all() (dicee.models.ComplEx method), 118
forward_k_vs_all() (dicee.models.complex.AConEx method), 75
forward_k_vs_all() (dicee.models.complex.ComplEx method), 76
forward_k_vs_all() (dicee.models.complex.ConEx method), 74
forward_k_vs_all() (dicee.models.ConEx method), 116
forward_k_vs_all() (dicee.models.ConvO method), 129
forward_k_vs_all() (dicee.models.ConvQ method), 123
forward_k_vs_all() (dicee.models.DeCaL method), 135
forward_k_vs_all() (dicee.models.DistMult method), 112
forward_k_vs_all() (dicee.models.DualE method), 146
forward_k_vs_all() (dicee.models.dualE.DualE method), 77
forward_k_vs_all() (dicee.models.Keci method), 132
forward_k_vs_all() (dicee.models.octonion.ACovO method), 86
forward_k_vs_all() (dicee.models.octonion.ConvO method), 85
forward_k_vs_all() (dicee.models.octonion.OMult method), 84
forward_k_vs_all() (dicee.models.OMult method), 128
forward_k_vs_all() (dicee.models.pykeen_models.PykeenKGE method), 87
forward_k_vs_all() (dicee.models.PykeenKGE method), 139
forward_k_vs_all() (dicee.models.QMult method), 123
forward_k_vs_all() (dicee.models.quaternion.ACovQ method), 90
forward_k_vs_all() (dicee.models.quaternion.ConvQ method), 90
forward_k_vs_all() (dicee.models.quaternion.QMult method), 89
forward_k_vs_all() (dicee.models.real.DistMult method), 91
forward_k_vs_all() (dicee.models.real.Shallom method), 91
forward_k_vs_all() (dicee.models.real.TransE method), 91
forward_k_vs_all() (dicee.models.Shallom method), 113
forward_k_vs_all() (dicee.models.TransE method), 113
forward_k_vs_all() (dicee.OMult method), 188
forward_k_vs_all() (dicee.PykeenKGE method), 190
forward_k_vs_all() (dicee.QMult method), 187
forward_k_vs_all() (dicee.Shallom method), 189
forward_k_vs_all() (dicee.TransE method), 176
forward_k_vs_sample() (dicee.AConEx method), 182
forward_k_vs_sample() (dicee.BaseKGE method), 195
forward_k_vs_sample() (dicee.ComplEx method), 182
forward_k_vs_sample() (dicee.ConEx method), 186

```

```

forward_k_vs_sample() (dicee.DistMult method), 173
forward_k_vs_sample() (dicee.Keci method), 176
forward_k_vs_sample() (dicee.models.AConEx method), 117
forward_k_vs_sample() (dicee.models.base_model.BaseKGE method), 65
forward_k_vs_sample() (dicee.models.BaseKGE method), 108, 112, 115, 120, 126, 139, 142
forward_k_vs_sample() (dicee.models.clifford.Keci method), 70
forward_k_vs_sample() (dicee.models.ComplEx method), 118
forward_k_vs_sample() (dicee.models.complex.AConEx method), 75
forward_k_vs_sample() (dicee.models.complex.ComplEx method), 76
forward_k_vs_sample() (dicee.models.complex.ConEx method), 75
forward_k_vs_sample() (dicee.models.ConEx method), 116
forward_k_vs_sample() (dicee.models.DistMult method), 112
forward_k_vs_sample() (dicee.models.Keci method), 132
forward_k_vs_sample() (dicee.models.pykeen_models.PykeenKGE method), 87
forward_k_vs_sample() (dicee.models.PykeenKGE method), 140
forward_k_vs_sample() (dicee.models.QMult method), 123
forward_k_vs_sample() (dicee.models.quaternion.QMult method), 89
forward_k_vs_sample() (dicee.models.real.DistMult method), 91
forward_k_vs_sample() (dicee.PykeenKGE method), 191
forward_k_vs_sample() (dicee.QMult method), 187
forward_k_vs_with_explicit() (dicee.Keci method), 175
forward_k_vs_with_explicit() (dicee.models.clifford.Keci method), 69
forward_k_vs_with_explicit() (dicee.models.Keci method), 132
forward_triples() (dicee.AConEx method), 182
forward_triples() (dicee.AConvO method), 183
forward_triples() (dicee.AConvQ method), 183
forward_triples() (dicee.BaseKGE method), 195
forward_triples() (dicee.ConEx method), 186
forward_triples() (dicee.ConvO method), 185
forward_triples() (dicee.ConvQ method), 184
forward_triples() (dicee.DeCaL method), 177
forward_triples() (dicee.DualE method), 180
forward_triples() (dicee.Keci method), 176
forward_triples() (dicee.LFMult method), 189
forward_triples() (dicee.models.AConEx method), 117
forward_triples() (dicee.models.AConvO method), 130
forward_triples() (dicee.models.AConvQ method), 124
forward_triples() (dicee.models.base_model.BaseKGE method), 65
forward_triples() (dicee.models.BaseKGE method), 108, 111, 115, 120, 126, 138, 142
forward_triples() (dicee.models.clifford.DeCaL method), 71
forward_triples() (dicee.models.clifford.Keci method), 70
forward_triples() (dicee.models.complex.AConEx method), 75
forward_triples() (dicee.models.complex.ConEx method), 74
forward_triples() (dicee.models.ConEx method), 116
forward_triples() (dicee.models.ConvO method), 129
forward_triples() (dicee.models.ConvQ method), 123
forward_triples() (dicee.models.DeCaL method), 134
forward_triples() (dicee.models.DualE method), 146
forward_triples() (dicee.models.dualE.DualE method), 77
forward_triples() (dicee.models.FMult method), 143
forward_triples() (dicee.models.FMult2 method), 144
forward_triples() (dicee.models.function_space.FMult method), 79
forward_triples() (dicee.models.function_space.FMult2 method), 80
forward_triples() (dicee.models.function_space.GFMult method), 79
forward_triples() (dicee.models.function_space.LFMult method), 81
forward_triples() (dicee.models.function_space.LFMult1 method), 80
forward_triples() (dicee.models.GFMult method), 143
forward_triples() (dicee.models.Keci method), 133
forward_triples() (dicee.models.LFMult method), 144
forward_triples() (dicee.models.LFMult1 method), 144
forward_triples() (dicee.models.octonion.AConvO method), 86
forward_triples() (dicee.models.octonion.ConvO method), 85
forward_triples() (dicee.models.Pyke method), 113
forward_triples() (dicee.models.pykeen_models.PykeenKGE method), 87
forward_triples() (dicee.models.PykeenKGE method), 140
forward_triples() (dicee.models.quaternion.AConvQ method), 90
forward_triples() (dicee.models.quaternion.ConvQ method), 90
forward_triples() (dicee.models.real.Pyke method), 92

```

```

forward_triples() (dicee.models.real.Shallom method), 91
forward_triples() (dicee.models.Shallom method), 113
forward_triples() (dicee.Pyke method), 172
forward_triples() (dicee.PykeenKGE method), 191
forward_triples() (dicee.Shallom method), 189
freeze_entity_embeddings (dicee.models.literal.LiteralEmbeddings attribute), 82, 83
frequency (dicee.callbacks.Perturb attribute), 27
from_pretrained() (dicee.models.transformers.GPT class method), 99
from_pretrained_model_write_embeddings_into_csv() (in module dicee), 197
from_pretrained_model_write_embeddings_into_csv() (in module dicee.static_funcs), 161
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), 144
function() (dicee.models.function_space.FMult2 method), 80

```

G

```

gamma (dicee.models.FMult attribute), 143
gamma (dicee.models.function_space.FMult attribute), 79
gate_residual (dicee.models.literal.LiteralEmbeddings attribute), 82
gated_residual_proj (dicee.models.literal.LiteralEmbeddings attribute), 83
gelu (dicee.models.transformers.MLP attribute), 96
gen_test (dicee.query_generator.QueryGenerator attribute), 147
gen_test (dicee.QueryGenerator attribute), 217
gen_valid (dicee.query_generator.QueryGenerator attribute), 147
gen_valid (dicee.QueryGenerator attribute), 217
generate() (dicee.BytE method), 192
generate() (dicee.KGE method), 199
generate() (dicee.knowledge_graph_embeddings.KGE method), 53
generate() (dicee.models.transformers.BytE method), 94
generate_queries() (dicee.query_generator.QueryGenerator method), 147
generate_queries() (dicee.QueryGenerator method), 218
get_aswa_state_dict() (dicee.callbacks.ASWA method), 25
get_bpe_head_and_relation_representation() (dicee.BaseKGE method), 195
get_bpe_head_and_relation_representation() (dicee.models.base_model.BaseKGE method), 66
get_bpe_head_and_relation_representation() (dicee.models.BaseKGE method), 109, 112, 115, 120, 126, 139, 142
get_bpe_token_representation() (dicee.abstracts.BaseInteractiveKGE method), 14
get_callbacks() (in module dicee.trainer.dice_trainer), 163
get_default_arguments() (in module dicee.analyse_experiments), 19
get_default_arguments() (in module dicee.scripts.index_serve), 156
get_default_arguments() (in module dicee.scripts.run), 158
get_ee_vocab() (in module dicee), 196
get_ee_vocab() (in module dicee.read_preprocess_save_load_kg.util), 152
get_ee_vocab() (in module dicee.static_funcs), 159
get_ee_vocab() (in module dicee.static_preprocess_funcs), 162
get_embeddings() (dicee.BaseKGE method), 195
get_embeddings() (dicee.EnsembleKGE method), 196
get_embeddings() (dicee.models.base_model.BaseKGE method), 66
get_embeddings() (dicee.models.BaseKGE method), 109, 112, 116, 120, 126, 139, 142
get_embeddings() (dicee.models.ensemble.EnsembleKGE method), 78
get_embeddings() (dicee.models.real.Shallom method), 91
get_embeddings() (dicee.models.Shallom method), 113
get_embeddings() (dicee.Shallom method), 189
get_entity_embeddings() (dicee.abstracts.BaseInteractiveKGE method), 15
get_entity_index() (dicee.abstracts.BaseInteractiveKGE method), 15
get_er_vocab() (in module dicee), 196
get_er_vocab() (in module dicee.read_preprocess_save_load_kg.util), 152
get_er_vocab() (in module dicee.static_funcs), 159
get_er_vocab() (in module dicee.static_preprocess_funcs), 162
get_eval_report() (dicee.abstracts.BaseInteractiveKGE method), 14
get_head_relation_representation() (dicee.BaseKGE method), 195
get_head_relation_representation() (dicee.models.base_model.BaseKGE method), 66
get_head_relation_representation() (dicee.models.BaseKGE method), 108, 112, 115, 120, 126, 139, 142
get_kronecker_triple_representation() (dicee.callbacks.KronE method), 26
get_num_params() (dicee.models.transformers.GPT method), 98
get_padded_bpe_triple_representation() (dicee.abstracts.BaseInteractiveKGE method), 14
get_queries() (dicee.query_generator.QueryGenerator method), 148

```

get_queries() (*dicee.QueryGenerator method*), 218
 get_re_vocab() (*in module dicee*), 196
 get_re_vocab() (*in module dicee.read_preprocess_save_load_kg.util*), 152
 get_re_vocab() (*in module dicee.static_funcs*), 159
 get_re_vocab() (*in module dicee.static_preprocess_funcs*), 162
 get_relation_embeddings() (*dicee.abstracts.BaseInteractiveKGE method*), 15
 get_relation_index() (*dicee.abstracts.BaseInteractiveKGE method*), 15
 get_sentence_representation() (*dicee.BaseKGE method*), 195
 get_sentence_representation() (*dicee.models.base_model.BaseKGE method*), 66
 get_sentence_representation() (*dicee.models.BaseKGE method*), 108, 112, 115, 120, 126, 139, 142
 get_transductive_entity_embeddings() (*dicee.KGE method*), 199
 get_transductive_entity_embeddings() (*dicee.knowledge_graph_embeddings.KGE method*), 53
 get_triple_representation() (*dicee.BaseKGE method*), 195
 get_triple_representation() (*dicee.models.base_model.BaseKGE method*), 65
 get_triple_representation() (*dicee.models.BaseKGE method*), 108, 112, 115, 120, 126, 139, 142
 GFMult (*class in dicee.models*), 143
 GFMult (*class in dicee.models.function_space*), 79
 global_rank (*dicee.abstracts.AbstractTrainer attribute*), 13
 global_rank (*dicee.trainer.torch_trainer_ddp.NodeTrainer attribute*), 167
 GPT (*class in dicee.models.transformers*), 98
 GPTConfig (*class in dicee.models.transformers*), 97
 gpus (*dicee.config.Namespace attribute*), 30
 gradient_accumulation_steps (*dicee.config.Namespace attribute*), 31
 ground_queries() (*dicee.query_generator.QueryGenerator method*), 147
 ground_queries() (*dicee.QueryGenerator method*), 217

H

hidden_dim (*dicee.models.literal.LiteralEmbeddings attribute*), 82
 hidden_dropout (*dicee.BaseKGE attribute*), 194
 hidden_dropout (*dicee.models.base_model.BaseKGE attribute*), 65
 hidden_dropout (*dicee.models.BaseKGE attribute*), 108, 111, 115, 119, 125, 138, 141
 hidden_dropout_rate (*dicee.BaseKGE attribute*), 194
 hidden_dropout_rate (*dicee.config.Namespace attribute*), 31
 hidden_dropout_rate (*dicee.models.base_model.BaseKGE attribute*), 64
 hidden_dropout_rate (*dicee.models.BaseKGE attribute*), 107, 110, 114, 119, 125, 137, 141
 hidden_normalizer (*dicee.BaseKGE attribute*), 194
 hidden_normalizer (*dicee.models.base_model.BaseKGE attribute*), 65
 hidden_normalizer (*dicee.models.BaseKGE attribute*), 108, 111, 114, 119, 125, 138, 141

I

IdentityClass (*class in dicee.models*), 109, 120, 126
 IdentityClass (*class in dicee.models.base_model*), 66
 idx_entity_to_bpe_shaped (*dicee.knowledge_graph.KG attribute*), 52
 index() (*in module dicee.scripts.index_serve*), 156
 index_triple() (*dicee.abstracts.BaseInteractiveKGE method*), 15
 init_dataloader() (*dicee.DICE_Trainer method*), 198
 init_dataloader() (*dicee.trainer.DICE_Trainer method*), 169
 init_dataloader() (*dicee.trainer.dice_trainer.DICE_Trainer method*), 164
 init_dataset() (*dicee.DICE_Trainer method*), 198
 init_dataset() (*dicee.trainer.DICE_Trainer method*), 169
 init_dataset() (*dicee.trainer.dice_trainer.DICE_Trainer method*), 164
 init_param (*dicee.config.Namespace attribute*), 31
 init_params_with_sanity_checking() (*dicee.BaseKGE method*), 195
 init_params_with_sanity_checking() (*dicee.models.base_model.BaseKGE method*), 65
 init_params_with_sanity_checking() (*dicee.models.BaseKGE method*), 108, 111, 115, 120, 126, 138, 142
 initial_eval_setting (*dicee.callbacks.ASWA attribute*), 24
 initialize_or_load_model() (*dicee.DICE_Trainer method*), 198
 initialize_or_load_model() (*dicee.trainer.DICE_Trainer method*), 169
 initialize_or_load_model() (*dicee.trainer.dice_trainer.DICE_Trainer method*), 164
 initialize_trainer() (*dicee.DICE_Trainer method*), 198
 initialize_trainer() (*dicee.trainer.DICE_Trainer method*), 169
 initialize_trainer() (*dicee.trainer.dice_trainer.DICE_Trainer method*), 164
 initialize_trainer() (*in module dicee.trainer.dice_trainer*), 163
 input_dp_ent_real (*dicee.BaseKGE attribute*), 194
 input_dp_ent_real (*dicee.models.base_model.BaseKGE attribute*), 65
 input_dp_ent_real (*dicee.models.BaseKGE attribute*), 108, 111, 115, 119, 125, 138, 141
 input_dp_rel_real (*dicee.BaseKGE attribute*), 194

```

input_dp_rel_real (dicee.models.base_model.BaseKGE attribute), 65
input_dp_rel_real (dicee.models.BaseKGE attribute), 108, 111, 115, 119, 125, 138, 141
input_dropout_rate (dicee.BaseKGE attribute), 194
input_dropout_rate (dicee.config.Namespace attribute), 31
input_dropout_rate (dicee.models.base_model.BaseKGE attribute), 64
input_dropout_rate (dicee.models.BaseKGE attribute), 107, 110, 114, 119, 125, 137, 141
InteractiveQueryDecomposition (class in dicee.abstracts), 16
initialize_model () (in module dicee), 197
initialize_model () (in module dicee.static_funcs), 160
is_continual_training (dicee.DICE_Trainer attribute), 198
is_continual_training (dicee.evaluator.Evaluator attribute), 48
is_continual_training (dicee.Execute attribute), 203
is_continual_training (dicee.executer.Execute attribute), 49
is_continual_training (dicee.trainer.DICE_Trainer attribute), 168
is_continual_training (dicee.trainer.dice_trainer.DICE_Trainer attribute), 163
is_global_zero (dicee.abstracts.AbstractTrainer attribute), 13
is_seen () (dicee.abstracts.BaseInteractiveKGE method), 15
is_sparql_endpoint_alive () (in module dicee.sanity_checkers), 155

```

K

```

k (dicee.models.FMult attribute), 142
k (dicee.models.FMult2 attribute), 143
k (dicee.models.function_space.FMult attribute), 79
k (dicee.models.function_space.FMult2 attribute), 79
k (dicee.models.function_space.GFMult attribute), 79
k (dicee.models.GFMult attribute), 143
k_fold_cross_validation () (dicee.DICE_Trainer method), 199
k_fold_cross_validation () (dicee.trainer.DICE_Trainer method), 169
k_fold_cross_validation () (dicee.trainer.dice_trainer.DICE_Trainer method), 164
k_vs_all_score () (dicee.ComplEx static method), 182
k_vs_all_score () (dicee.DistMult method), 173
k_vs_all_score () (dicee.Keci method), 175
k_vs_all_score () (dicee.models.clifford.Keci method), 69
k_vs_all_score () (dicee.models.ComplEx static method), 117
k_vs_all_score () (dicee.models.complex.ComplEx static method), 76
k_vs_all_score () (dicee.models.DistMult method), 112
k_vs_all_score () (dicee.models.Keci method), 132
k_vs_all_score () (dicee.models.octonion.OMult method), 84
k_vs_all_score () (dicee.models.OMult method), 128
k_vs_all_score () (dicee.models.QMult method), 122
k_vs_all_score () (dicee.models.quaternion.QMult method), 89
k_vs_all_score () (dicee.models.real.DistMult method), 91
k_vs_all_score () (dicee.OMult method), 188
k_vs_all_score () (dicee.QMult method), 187
Keci (class in dicee), 173
Keci (class in dicee.models), 130
Keci (class in dicee.models.clifford), 67
kernel_size (dicee.BaseKGE attribute), 194
kernel_size (dicee.config.Namespace attribute), 31
kernel_size (dicee.models.base_model.BaseKGE attribute), 64
kernel_size (dicee.models.BaseKGE attribute), 107, 111, 114, 119, 125, 138, 141
KG (class in dicee.knowledge_graph), 51
kg (dicee.callbacks.PseudoLabellingCallback attribute), 24
kg (dicee.read_preprocess_save_load_kg.LoadSaveToDisk attribute), 154
kg (dicee.read_preprocess_save_load_kg.PreprocessKG attribute), 153
kg (dicee.read_preprocess_save_load_kg.preprocess.PreprocessKG attribute), 148
kg (dicee.read_preprocess_save_load_kg.read_from_disk.ReadFromDisk attribute), 149
kg (dicee.read_preprocess_save_load_kg.ReadFromDisk attribute), 154
kg (dicee.read_preprocess_save_load_kg.save_load_disk.LoadSaveToDisk attribute), 150
KGE (class in dicee), 199
KGE (class in dicee.knowledge_graph_embeddings), 53
KGESaveCallback (class in dicee.callbacks), 22
knowledge_graph (dicee.Execute attribute), 203
knowledge_graph (dicee.executer.Execute attribute), 50
KronE (class in dicee.callbacks), 26
KvsAll (class in dicee), 206
KvsAll (class in dicee.dataset_classes), 35

```

kvsall_score() (*dicee.DualE method*), 180
 kvsall_score() (*dicee.models.DualE method*), 146
 kvsall_score() (*dicee.models.dualE.DualE method*), 77
 KvsSampleDataset (*class in dicee*), 209
 KvsSampleDataset (*class in dicee.dataset_classes*), 39

L

label_smoothing_rate (*dicee.AllvsAll attribute*), 207
 label_smoothing_rate (*dicee.config.Namespace attribute*), 31
 label_smoothing_rate (*dicee.dataset_classes.AllvsAll attribute*), 37
 label_smoothing_rate (*dicee.dataset_classes.KvsAll attribute*), 36
 label_smoothing_rate (*dicee.dataset_classes.KvsSampleDataset attribute*), 39
 label_smoothing_rate (*dicee.dataset_classes.OnevsSample attribute*), 38
 label_smoothing_rate (*dicee.dataset_classes.TriplePredictionDataset attribute*), 40
 label_smoothing_rate (*dicee.KvsAll attribute*), 207
 label_smoothing_rate (*dicee.KvsSampleDataset attribute*), 210
 label_smoothing_rate (*dicee.OnevsSample attribute*), 208, 209
 label_smoothing_rate (*dicee.TriplePredictionDataset attribute*), 211
 layer_norm (*dicee.models.literal.LiteralEmbeddings attribute*), 83
 LayerNorm (*class in dicee.models.transformers*), 95
 learning_rate (*dicee.BaseKGE attribute*), 194
 learning_rate (*dicee.models.base_model.BaseKGE attribute*), 64
 learning_rate (*dicee.models.BaseKGE attribute*), 107, 110, 114, 119, 125, 137, 141
 length (*dicee.dataset_classes.NegSampleDataset attribute*), 40
 length (*dicee.dataset_classes.TriplePredictionDataset attribute*), 41
 length (*dicee.NegSampleDataset attribute*), 210
 length (*dicee.TriplePredictionDataset attribute*), 211
 level (*dicee.callbacks.Perturb attribute*), 27
 LFMult (*class in dicee*), 189
 LFMult (*class in dicee.models*), 144
 LFMult (*class in dicee.models.function_space*), 80
 LFMult1 (*class in dicee.models*), 144
 LFMult1 (*class in dicee.models.function_space*), 80
 linear() (*dicee.LFMult method*), 189
 linear() (*dicee.models.function_space.LFMult method*), 81
 linear() (*dicee.models.LFMult method*), 145
 list2tuple() (*dicee.query_generator.QueryGenerator method*), 147
 list2tuple() (*dicee.QueryGenerator method*), 217
 LiteralDataset (*class in dicee*), 215
 LiteralDataset (*class in dicee.dataset_classes*), 44
 LiteralEmbeddings (*class in dicee.models.literal*), 82
 lm_head (*dicee.BytE attribute*), 192
 lm_head (*dicee.models.transformers.BytE attribute*), 93
 lm_head (*dicee.models.transformers.GPT attribute*), 98
 ln_1 (*dicee.models.transformers.Block attribute*), 97
 ln_2 (*dicee.models.transformers.Block attribute*), 97
 load() (*dicee.read_preprocess_save_load_kg.LoadSaveToDisk method*), 154
 load() (*dicee.read_preprocess_save_load_kg.save_load_disk.LoadSaveToDisk method*), 150
 load_and_validate_literal_data() (*dicee.dataset_classes.LiteralDataset static method*), 46
 load_and_validate_literal_data() (*dicee.LiteralDataset static method*), 216
 load_json() (*in module dicee*), 197
 load_json() (*in module dicee.static_funcs*), 160
 load_model() (*in module dicee*), 196
 load_model() (*in module dicee.static_funcs*), 160
 load_model_ensemble() (*in module dicee*), 196
 load_model_ensemble() (*in module dicee.static_funcs*), 160
 load_numpy() (*in module dicee*), 197
 load_numpy() (*in module dicee.static_funcs*), 161
 load_numpy_ndarray() (*in module dicee.read_preprocess_save_load_kg.util*), 153
 load_pickle() (*in module dicee*), 196
 load_pickle() (*in module dicee.read_preprocess_save_load_kg.util*), 153
 load_pickle() (*in module dicee.static_funcs*), 160
 load_queries() (*dicee.query_generator.QueryGenerator method*), 148
 load_queries() (*dicee.QueryGenerator method*), 218
 load_queries_and_answers() (*dicee.query_generator.QueryGenerator static method*), 148
 load_queries_and_answers() (*dicee.QueryGenerator static method*), 218
 load_term_mapping() (*in module dicee*), 196, 204

load_term_mapping() (*in module dicee.static_funcs*), 160
 load_term_mapping() (*in module dicee.trainer.dice_trainer*), 163
 load_with_pandas() (*in module dicee.read_preprocess_save_load_kg.util*), 153
 loader_backend (*dicee.dataset_classes.LiteralDataset* attribute), 45
 loader_backend (*dicee.LiteralDataset* attribute), 216
 LoadSaveToDisk (*class in dicee.read_preprocess_save_load_kg*), 154
 LoadSaveToDisk (*class in dicee.read_preprocess_save_load_kg.save_load_disk*), 150
 local_rank (*dicee.abstracts.AbstractTrainer* attribute), 13
 local_rank (*dicee.trainer.torch_trainer_ddp.NodeTrainer* attribute), 167
 loss (*dicee.BaseKGE* attribute), 194
 loss (*dicee.models.base_model.BaseKGE* attribute), 64
 loss (*dicee.models.BaseKGE* attribute), 107, 111, 114, 119, 125, 138, 141
 loss_func (*dicee.trainer.torch_trainer_ddp.NodeTrainer* attribute), 168
 loss_function (*dicee.trainer.torch_trainer.TorchTrainer* attribute), 166
 loss_function() (*dicee.BytE* method), 192
 loss_function() (*dicee.models.base_model.BaseKGELightning* method), 59
 loss_function() (*dicee.models.BaseKGELightning* method), 102
 loss_function() (*dicee.models.transformers.BytE* method), 93
 loss_history (*dicee.BaseKGE* attribute), 194
 loss_history (*dicee.models.base_model.BaseKGE* attribute), 65
 loss_history (*dicee.models.BaseKGE* attribute), 108, 111, 115, 119, 125, 138, 141
 loss_history (*dicee.models.pykeen_models.PykeenKGE* attribute), 86
 loss_history (*dicee.models.PykeenKGE* attribute), 139
 loss_history (*dicee.PykeenKGE* attribute), 190
 loss_history (*dicee.trainer.torch_trainer_ddp.NodeTrainer* attribute), 168
 lr (*dicee.analyse_experiments.Experiment* attribute), 19
 lr (*dicee.config.Namespace* attribute), 30
 lr_init (*dicee.callbacks.SWA* attribute), 29
 lr_lambda (*dicee.callbacks.LRScheduler* attribute), 28
 LRScheduler (*class in dicee.callbacks*), 28

M

m (*dicee.LFMult* attribute), 189
 m (*dicee.models.function_space.LFMult* attribute), 80
 m (*dicee.models.LFMult* attribute), 144
 main() (*in module dicee.scripts.index_serve*), 158
 main() (*in module dicee.scripts.run*), 158
 make_iterable_verbose() (*in module dicee.static_funcs_training*), 161
 make_iterable_verbose() (*in module dicee.trainer.torch_trainer_ddp*), 167
 mapping_from_first_two_cols_to_third() (*in module dicee*), 204
 mapping_from_first_two_cols_to_third() (*in module dicee.static_preprocess_funcs*), 163
 margin (*dicee.models.Pyke* attribute), 113
 margin (*dicee.models.real.Pyke* attribute), 92
 margin (*dicee.models.real.TransE* attribute), 91
 margin (*dicee.models.TransE* attribute), 112
 margin (*dicee.Pyke* attribute), 172
 margin (*dicee.TransE* attribute), 176
 max_ans_num (*dicee.query_generator.QueryGenerator* attribute), 147
 max_ans_num (*dicee.QueryGenerator* attribute), 217
 max_epochs (*dicee.callbacks.KGESaveCallback* attribute), 23
 max_epochs (*dicee.callbacks.PeriodicEvalCallback* attribute), 27
 max_epochs (*dicee.callbacks.SWA* attribute), 29
 max_length_subword_tokens (*dicee.BaseKGE* attribute), 194
 max_length_subword_tokens (*dicee.knowledge_graph.KG* attribute), 52
 max_length_subword_tokens (*dicee.models.base_model.BaseKGE* attribute), 65
 max_length_subword_tokens (*dicee.models.BaseKGE* attribute), 108, 111, 115, 119, 125, 138, 141
 max_num_of_classes (*dicee.dataset_classes.KvsSampleDataset* attribute), 39
 max_num_of_classes (*dicee.KvsSampleDataset* attribute), 210
 mem_of_model() (*dicee.EnsembleKGE* method), 196
 mem_of_model() (*dicee.models.base_model.BaseKGELightning* method), 58
 mem_of_model() (*dicee.models.BaseKGELightning* method), 101
 mem_of_model() (*dicee.models.ensemble.EnsembleKGE* method), 78
 method (*dicee.callbacks.Perturb* attribute), 27
 MLP (*class in dicee.models.transformers*), 96
 mlp (*dicee.models.transformers.Block* attribute), 97
 mode (*dicee.query_generator.QueryGenerator* attribute), 147
 mode (*dicee.QueryGenerator* attribute), 217

```

model (dicee.config.Namespace attribute), 30
model (dicee.models.pykeen_models.PykeenKGE attribute), 86
model (dicee.models.PykeenKGE attribute), 139
model (dicee.PykeenKGE attribute), 190
model (dicee.trainer.torch_trainer_ddp.NodeTrainer attribute), 168
model (dicee.trainer.torch_trainer.TorchTrainer attribute), 166
model_kwarg (dicee.models.pykeen_models.PykeenKGE attribute), 86
model_kwarg (dicee.models.PykeenKGE attribute), 139
model_kwarg (dicee.PykeenKGE attribute), 190
model_name (dicee.analyse_experiments.Experiment attribute), 19
module
    dicee, 12
    dicee.__main__, 12
    dicee.abstracts, 12
    dicee.analyse_experiments, 19
    dicee.callbacks, 20
    dicee.config, 29
    dicee.dataset_classes, 32
    dicee.eval_static_funcs, 46
    dicee.evaluator, 48
    dicee.executor, 49
    dicee.knowledge_graph, 51
    dicee.knowledge_graph_embeddings, 53
    dicee.models, 56
    dicee.models.adopt, 56
    dicee.models.base_model, 58
    dicee.models.clifford, 67
    dicee.models.complex, 74
    dicee.models.dualE, 76
    dicee.models.ensemble, 77
    dicee.models.function_space, 78
    dicee.models.literal, 82
    dicee.models.octonion, 83
    dicee.models.pykeen_models, 86
    dicee.models.quaternion, 87
    dicee.models.real, 90
    dicee.models.static_funcs, 92
    dicee.models.transformers, 92
    dicee.query_generator, 146
    dicee.read_preprocess_save_load_kg, 148
    dicee.read_preprocess_save_load_kg.preprocess, 148
    dicee.read_preprocess_save_load_kg.read_from_disk, 149
    dicee.read_preprocess_save_load_kg.save_load_disk, 149
    dicee.read_preprocess_save_load_kg.util, 150
    dicee.sanity_checkers, 154
    dicee.scripts, 155
    dicee.scripts.index_serve, 155
    dicee.scripts.run, 158
    dicee.static_funcs, 158
    dicee.static_funcs_training, 161
    dicee.static_preprocess_funcs, 162
    dicee.trainer, 163
    dicee.trainer.dice_trainer, 163
    dicee.trainer.model_parallelism, 165
    dicee.trainer.torch_trainer, 165
    dicee.trainer.torch_trainer_ddp, 167
modules() (dicee.EnsembleKGE method), 196
modules() (dicee.models.ensemble.EnsembleKGE method), 78
moving_average() (dicee.callbacks.SWA method), 29
MultiClassClassificationDataset (class in dicee), 205
MultiClassClassificationDataset (class in dicee.dataset_classes), 34
MultiLabelDataset (class in dicee), 205
MultiLabelDataset (class in dicee.dataset_classes), 34

```

N

n (dicee.models.FMult2 attribute), 143
n (dicee.models.function_space.FMult2 attribute), 79

n_embd (*dicee.models.transformers.CausalSelfAttention* attribute), 96
n_embd (*dicee.models.transformers.GPTConfig* attribute), 98
n_epochs_eval_model (*dicee.callbacks.PeriodicEvalCallback* attribute), 27
n_epochs_eval_model (*dicee.config.Namespace* attribute), 32
n_head (*dicee.models.transformers.CausalSelfAttention* attribute), 96
n_head (*dicee.models.transformers.GPTConfig* attribute), 98
n_layer (*dicee.models.transformers.GPTConfig* attribute), 97
n_layers (*dicee.models.FMul2* attribute), 143
n_layers (*dicee.models.function_space.FMul2* attribute), 79
name (*dicee.abstracts.BaseInteractiveKGE* property), 15
name (*dicee.AConEx* attribute), 182
name (*dicee.AConvO* attribute), 182
name (*dicee.AConvQ* attribute), 183
name (*dicee.BytE* attribute), 191
name (*dicee.CKeci* attribute), 173
name (*dicee.ComplEx* attribute), 182
name (*dicee.ConEx* attribute), 185
name (*dicee.ConvO* attribute), 185
name (*dicee.ConvQ* attribute), 184
name (*dicee.DeCaL* attribute), 177
name (*dicee.DistMult* attribute), 173
name (*dicee.DualE* attribute), 180
name (*dicee.EnsembleKGE* attribute), 195
name (*dicee.Keci* attribute), 174
name (*dicee.LFMult* attribute), 189
name (*dicee.models.AConEx* attribute), 116
name (*dicee.models.AConvO* attribute), 129
name (*dicee.models.AConvQ* attribute), 123
name (*dicee.models.CKeci* attribute), 133
name (*dicee.models.clifford.CKeci* attribute), 70
name (*dicee.models.clifford.DeCaL* attribute), 71
name (*dicee.models.clifford.Keci* attribute), 67
name (*dicee.models.ComplEx* attribute), 117
name (*dicee.models.complex.AConEx* attribute), 75
name (*dicee.models.complex.ComplEx* attribute), 76
name (*dicee.models.complex.ConEx* attribute), 74
name (*dicee.models.ConEx* attribute), 116
name (*dicee.models.ConvO* attribute), 129
name (*dicee.models.ConvQ* attribute), 123
name (*dicee.models.DeCaL* attribute), 134
name (*dicee.models.DistMult* attribute), 112
name (*dicee.models.DualE* attribute), 145
name (*dicee.models.dualE.DualE* attribute), 76
name (*dicee.models.ensemble.EnsembleKGE* attribute), 78
name (*dicee.models.FMult* attribute), 142
name (*dicee.models.FMul2* attribute), 143
name (*dicee.models.function_space.FMult* attribute), 78
name (*dicee.models.function_space.FMul2* attribute), 79
name (*dicee.models.function_space.GFMult* attribute), 79
name (*dicee.models.function_space.LFMult* attribute), 80
name (*dicee.models.function_space.LFMult1* attribute), 80
name (*dicee.models.GFMult* attribute), 143
name (*dicee.models.Keci* attribute), 130
name (*dicee.models.LFMult* attribute), 144
name (*dicee.models.LFMult1* attribute), 144
name (*dicee.models.octonion.AConvO* attribute), 86
name (*dicee.models.octonion.ConvO* attribute), 85
name (*dicee.models.octonion.OMult* attribute), 84
name (*dicee.models.OMult* attribute), 128
name (*dicee.models.Pyke* attribute), 113
name (*dicee.models.pykeen_models.PykeenKGE* attribute), 86
name (*dicee.models.PykeenKGE* attribute), 139
name (*dicee.models.QMult* attribute), 122
name (*dicee.models.quaternion.AConvQ* attribute), 90
name (*dicee.models.quaternion.ConvQ* attribute), 89
name (*dicee.models.quaternion.QMult* attribute), 88
name (*dicee.models.real.DistMult* attribute), 91
name (*dicee.models.real.Pyke* attribute), 92

name (*dicee.models.real.Shallom attribute*), 91
 name (*dicee.models.real.TransE attribute*), 91
 name (*dicee.models.Shallom attribute*), 113
 name (*dicee.models.TransE attribute*), 112
 name (*dicee.models.transformers.BytE attribute*), 93
 name (*dicee.OMult attribute*), 188
 name (*dicee.Pyke attribute*), 172
 name (*dicee.PykeenKGE attribute*), 190
 name (*dicee.QMult attribute*), 187
 name (*dicee.Shallom attribute*), 188
 name (*dicee.TransE attribute*), 176
 named_children () (*dicee.EnsembleKGE method*), 196
 named_children () (*dicee.models.ensemble.EnsembleKGE method*), 78
 Namespace (*class in dicee.config*), 29
 neg_ratio (*dicee.BPE_NegativeSamplingDataset attribute*), 204
 neg_ratio (*dicee.config.Namespace attribute*), 30
 neg_ratio (*dicee.dataset_classes.BPE_NegativeSamplingDataset attribute*), 34
 neg_ratio (*dicee.dataset_classes.KvsSampleDataset attribute*), 39
 neg_ratio (*dicee.KvsSampleDataset attribute*), 210
 neg_sample_ratio (*dicee.CVDataModule attribute*), 212
 neg_sample_ratio (*dicee.dataset_classes.CVDataModule attribute*), 41
 neg_sample_ratio (*dicee.dataset_classes.NegSampleDataset attribute*), 40
 neg_sample_ratio (*dicee.dataset_classes.OnevsSample attribute*), 38
 neg_sample_ratio (*dicee.dataset_classes.TriplePredictionDataset attribute*), 41
 neg_sample_ratio (*dicee.NegSampleDataset attribute*), 210
 neg_sample_ratio (*dicee.OnevsSample attribute*), 208, 209
 neg_sample_ratio (*dicee.TriplePredictionDataset attribute*), 211
 negnorm () (*dicee.abstracts.InteractiveQueryDecomposition method*), 16
 NegSampleDataset (*class in dicee*), 210
 NegSampleDataset (*class in dicee.dataset_classes*), 39
 neural_searcher (*in module dicee.scripts.index_serve*), 156
 NeuralSearcher (*class in dicee.scripts.index_serve*), 156
 NodeTrainer (*class in dicee.trainer.torch_trainer_ddp*), 167
 norm_fc1 (*dicee.AConEx attribute*), 182
 norm_fc1 (*dicee.AConvO attribute*), 183
 norm_fc1 (*dicee.ConEx attribute*), 186
 norm_fc1 (*dicee.ConvO attribute*), 185
 norm_fc1 (*dicee.models.AConEx attribute*), 116
 norm_fc1 (*dicee.models.AConvO attribute*), 129
 norm_fc1 (*dicee.models.complex.AConEx attribute*), 75
 norm_fc1 (*dicee.models.complex.ConEx attribute*), 74
 norm_fc1 (*dicee.models.ConEx attribute*), 116
 norm_fc1 (*dicee.models.ConvO attribute*), 129
 norm_fc1 (*dicee.models.octonion.AConvO attribute*), 86
 norm_fc1 (*dicee.models.octonion.ConvO attribute*), 85
 normalization (*dicee.analyse_experiments.Experiment attribute*), 20
 normalization (*dicee.config.Namespace attribute*), 31
 normalization (*dicee.dataset_classes.LiteralDataset attribute*), 44
 normalization (*dicee.LiteralDataset attribute*), 215
 normalization_params (*dicee.dataset_classes.LiteralDataset attribute*), 45
 normalization_params (*dicee.LiteralDataset attribute*), 215, 216
 normalization_type (*dicee.dataset_classes.LiteralDataset attribute*), 45
 normalization_type (*dicee.LiteralDataset attribute*), 216
 normalize_head_entity_embeddings (*dicee.BaseKGE attribute*), 194
 normalize_head_entity_embeddings (*dicee.models.base_model.BaseKGE attribute*), 65
 normalize_head_entity_embeddings (*dicee.models.BaseKGE attribute*), 108, 111, 114, 119, 125, 138, 141
 normalize_relation_embeddings (*dicee.BaseKGE attribute*), 194
 normalize_relation_embeddings (*dicee.models.base_model.BaseKGE attribute*), 65
 normalize_relation_embeddings (*dicee.models.BaseKGE attribute*), 108, 111, 114, 119, 125, 138, 141
 normalize_tail_entity_embeddings (*dicee.BaseKGE attribute*), 194
 normalize_tail_entity_embeddings (*dicee.models.base_model.BaseKGE attribute*), 65
 normalize_tail_entity_embeddings (*dicee.models.BaseKGE attribute*), 108, 111, 114, 119, 125, 138, 141
 normalizer_class (*dicee.BaseKGE attribute*), 194
 normalizer_class (*dicee.models.base_model.BaseKGE attribute*), 65
 normalizer_class (*dicee.models.BaseKGE attribute*), 107, 111, 114, 119, 125, 138, 141
 num_bpe_entities (*dicee.BPE_NegativeSamplingDataset attribute*), 204
 num_bpe_entities (*dicee.dataset_classes.BPE_NegativeSamplingDataset attribute*), 34
 num_bpe_entities (*dicee.knowledge_graph.KG attribute*), 52

num_core (*dicee.config.Namespace* attribute), 31
 num_data_properties (*dicee.dataset_classes.LiteralDataset* attribute), 45
 num_data_properties (*dicee.LiteralDataset* attribute), 216
 num_datapoints (*dicee.BPE_NegativeSamplingDataset* attribute), 204
 num_datapoints (*dicee.dataset_classes.BPE_NegativeSamplingDataset* attribute), 34
 num_datapoints (*dicee.dataset_classes.MultiLabelDataset* attribute), 34
 num_datapoints (*dicee.MultiLabelDataset* attribute), 205
 num_ent (*dicee.DualE* attribute), 180
 num_ent (*dicee.models.DualE* attribute), 146
 num_ent (*dicee.models.dualE.DualE* attribute), 77
 num_entities (*dicee.BaseKGE* attribute), 194
 num_entities (*dicee.CVDataModule* attribute), 212
 num_entities (*dicee.dataset_classes.CVDataModule* attribute), 41
 num_entities (*dicee.dataset_classes.KvsSampleDataset* attribute), 39
 num_entities (*dicee.dataset_classes.LiteralDataset* attribute), 45
 num_entities (*dicee.dataset_classes.NegSampleDataset* attribute), 40
 num_entities (*dicee.dataset_classes.OnevsSample* attribute), 37, 38
 num_entities (*dicee.dataset_classes.TriplePredictionDataset* attribute), 41
 num_entities (*dicee.evaluator.Evaluator* attribute), 48
 num_entities (*dicee.knowledge_graph.KG* attribute), 51
 num_entities (*dicee.KvsSampleDataset* attribute), 210
 num_entities (*dicee.LiteralDataset* attribute), 216
 num_entities (*dicee.models.base_model.BaseKGE* attribute), 64
 num_entities (*dicee.models.BaseKGE* attribute), 107, 110, 114, 118, 125, 137, 141
 num_entities (*dicee.NegSampleDataset* attribute), 210
 num_entities (*dicee.OnevsSample* attribute), 208, 209
 num_entities (*dicee.TriplePredictionDataset* attribute), 211
 num_epochs (*dicee.abstracts.AbstractPPECallback* attribute), 17
 num_epochs (*dicee.analyse_experiments.Experiment* attribute), 19
 num_epochs (*dicee.callbacks.ASWA* attribute), 24
 num_epochs (*dicee.config.Namespace* attribute), 30
 num_epochs (*dicee.trainer.torch_trainer_dlp.NodeTrainer* attribute), 168
 num_folds_for_cv (*dicee.config.Namespace* attribute), 31
 num_of_data_points (*dicee.dataset_classes.MultiClassClassificationDataset* attribute), 35
 num_of_data_points (*dicee.MultiClassClassificationDataset* attribute), 206
 num_of_data_properties (*dicee.models.literal.LiteralEmbeddings* attribute), 82
 num_of_epochs (*dicee.callbacks.PseudoLabellingCallback* attribute), 24
 num_of_output_channels (*dicee.BaseKGE* attribute), 194
 num_of_output_channels (*dicee.config.Namespace* attribute), 31
 num_of_output_channels (*dicee.models.base_model.BaseKGE* attribute), 64
 num_of_output_channels (*dicee.models.BaseKGE* attribute), 107, 111, 114, 119, 125, 138, 141
 num_params (*dicee.analyse_experiments.Experiment* attribute), 19
 num_relations (*dicee.BaseKGE* attribute), 194
 num_relations (*dicee.CVDataModule* attribute), 212
 num_relations (*dicee.dataset_classes.CVDataModule* attribute), 41
 num_relations (*dicee.dataset_classes.NegSampleDataset* attribute), 40
 num_relations (*dicee.dataset_classes.OnevsSample* attribute), 38
 num_relations (*dicee.dataset_classes.TriplePredictionDataset* attribute), 41
 num_relations (*dicee.evaluator.Evaluator* attribute), 48
 num_relations (*dicee.knowledge_graph.KG* attribute), 51
 num_relations (*dicee.models.base_model.BaseKGE* attribute), 64
 num_relations (*dicee.models.BaseKGE* attribute), 107, 110, 114, 119, 125, 137, 141
 num_relations (*dicee.NegSampleDataset* attribute), 210
 num_relations (*dicee.OnevsSample* attribute), 208, 209
 num_relations (*dicee.TriplePredictionDataset* attribute), 211
 num_sample (*dicee.models.FMult* attribute), 142
 num_sample (*dicee.models.function_space.FMult* attribute), 79
 num_sample (*dicee.models.function_space.GFMult* attribute), 79
 num_sample (*dicee.models.GFMult* attribute), 143
 num_tokens (*dicee.BaseKGE* attribute), 194
 num_tokens (*dicee.knowledge_graph.KG* attribute), 52
 num_tokens (*dicee.models.base_model.BaseKGE* attribute), 64
 num_tokens (*dicee.models.BaseKGE* attribute), 107, 110, 114, 119, 125, 137, 141
 num_workers (*dicee.CVDataModule* attribute), 212
 num_workers (*dicee.dataset_classes.CVDataModule* attribute), 41
 numpy_data_type_changer () (in module *dicee*), 197
 numpy_data_type_changer () (in module *dicee.static_funcs*), 160

O

octonion_mul () (in module dicee.models), 127
octonion_mul () (in module dicee.models.octonion), 83
octonion_mul_norm () (in module dicee.models), 127
octonion_mul_norm () (in module dicee.models.octonion), 83
octonion_normalizer () (dicee.AConvO static method), 183
octonion_normalizer () (dicee.ConvO static method), 185
octonion_normalizer () (dicee.models.AConvO static method), 129
octonion_normalizer () (dicee.models.ConvO static method), 129
octonion_normalizer () (dicee.models.octonion.AConvO static method), 86
octonion_normalizer () (dicee.models.octonion.ConvO static method), 85
octonion_normalizer () (dicee.models.octonion.OMult static method), 84
octonion_normalizer () (dicee.models.OMult static method), 128
octonion_normalizer () (dicee.OMult static method), 188
OMult (class in dicee), 187
OMult (class in dicee.models), 127
OMult (class in dicee.models.octonion), 83
on_epoch_end () (dicee.callbacks.KGESaveCallback method), 24
on_epoch_end () (dicee.callbacks.PseudoLabellingCallback method), 24
on_fit_end () (dicee.abstracts.AbstractCallback method), 17
on_fit_end () (dicee.abstracts.AbstractPPECallback method), 18
on_fit_end () (dicee.abstracts.AbstractTrainer method), 13
on_fit_end () (dicee.callbacks.AccumulateEpochLossCallback method), 21
on_fit_end () (dicee.callbacks.ASWA method), 24
on_fit_end () (dicee.callbacks.Eval method), 26
on_fit_end () (dicee.callbacks.KGESaveCallback method), 23
on_fit_end () (dicee.callbacks.LRScheduler method), 28
on_fit_end () (dicee.callbacks.PeriodicEvalCallback method), 28
on_fit_end () (dicee.callbacks.PrintCallback method), 22
on_fit_end () (dicee.callbacks.SWA method), 29
on_fit_start () (dicee.abstracts.AbstractCallback method), 16
on_fit_start () (dicee.abstracts.AbstractPPECallback method), 18
on_fit_start () (dicee.abstracts.AbstractTrainer method), 13
on_fit_start () (dicee.callbacks.Eval method), 25
on_fit_start () (dicee.callbacks.KGESaveCallback method), 23
on_fit_start () (dicee.callbacks.KronE method), 27
on_fit_start () (dicee.callbacks.PrintCallback method), 22
on_fit_start () (dicee.callbacks.SWA method), 29
on_init_end () (dicee.abstracts.AbstractCallback method), 16
on_init_start () (dicee.abstracts.AbstractCallback method), 16
on_train_batch_end () (dicee.abstracts.AbstractCallback method), 17
on_train_batch_end () (dicee.abstracts.AbstractTrainer method), 13
on_train_batch_end () (dicee.callbacks.Eval method), 26
on_train_batch_end () (dicee.callbacks.KGESaveCallback method), 23
on_train_batch_end () (dicee.callbacks.LRScheduler method), 28
on_train_batch_end () (dicee.callbacks.PrintCallback method), 22
on_train_batch_start () (dicee.callbacks.Perturb method), 27
on_train_epoch_end () (dicee.abstracts.AbstractCallback method), 17
on_train_epoch_end () (dicee.abstracts.AbstractTrainer method), 13
on_train_epoch_end () (dicee.callbacks.ASWA method), 25
on_train_epoch_end () (dicee.callbacks.Eval method), 26
on_train_epoch_end () (dicee.callbacks.KGESaveCallback method), 23
on_train_epoch_end () (dicee.callbacks.PeriodicEvalCallback method), 28
on_train_epoch_end () (dicee.callbacks.PrintCallback method), 22
on_train_epoch_end () (dicee.callbacks.SWA method), 29
on_train_epoch_end () (dicee.models.base_model.BaseKGELightning method), 60
on_train_epoch_end () (dicee.models.BaseKGELightning method), 102
on_train_epoch_start () (dicee.abstracts.AbstractTrainer method), 13
on_train_epoch_start () (dicee.callbacks.SWA method), 29
on_train_start () (dicee.callbacks.LRScheduler method), 28
OnevsAllDataset (class in dicee), 206
OnevsAllDataset (class in dicee.dataset_classes), 35
OnevsSample (class in dicee), 208
OnevsSample (class in dicee.dataset_classes), 37
optim (dicee.config.Namespace attribute), 30
optimizer (dicee.trainer.torch_trainer_ddp.NodeTrainer attribute), 167
optimizer (dicee.trainer.torch_trainer.TorchTrainer attribute), 166
optimizer_name (dicee.BaseKGE attribute), 194

optimizer_name (*dicee.models.base_model.BaseKGE* attribute), 64
 optimizer_name (*dicee.models.BaseKGE* attribute), 107, 110, 114, 119, 125, 137, 141
 ordered_bpe_entities (*dicee.BPE_NegativeSamplingDataset* attribute), 204
 ordered_bpe_entities (*dicee.dataset_classes.BPE_NegativeSamplingDataset* attribute), 34
 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), 177
 p (*dicee.Keci* attribute), 174
 p (*dicee.models.clifford.DeCaL* attribute), 71
 p (*dicee.models.clifford.Keci* attribute), 67
 p (*dicee.models.DeCaL* attribute), 134
 p (*dicee.models.Keci* attribute), 130
 padding (*dicee.knowledge_graph.KG* attribute), 52
 pandas_dataframe_indexer() (in module *dicee.read_preprocess_save_load_kg.util*), 152
 param_init (*dicee.BaseKGE* attribute), 194
 param_init (*dicee.models.base_model.BaseKGE* attribute), 65
 param_init (*dicee.models.BaseKGE* attribute), 108, 111, 115, 119, 125, 138, 141
 parameters() (*dicee.abstracts.BaseInteractiveKGE* method), 16
 parameters() (*dicee.EnsembleKGE* method), 196
 parameters() (*dicee.models.ensemble.EnsembleKGE* method), 78
 path (*dicee.abstracts.AbstractPPECallback* attribute), 17
 path (*dicee.callbacks.AccumulateEpochLossCallback* attribute), 21
 path (*dicee.callbacks.ASWA* attribute), 24
 path (*dicee.callbacks.Eval* attribute), 25
 path (*dicee.callbacks.KGESaveCallback* attribute), 23
 path_dataset_folder (*dicee.analyse_experiments.Experiment* attribute), 19
 path_for_deserialization (*dicee.knowledge_graph.KG* attribute), 52
 path_for_serialization (*dicee.knowledge_graph.KG* attribute), 52
 path_single_kg (*dicee.config.Namespace* attribute), 30
 path_single_kg (*dicee.knowledge_graph.KG* attribute), 51
 path_to_store_single_run (*dicee.config.Namespace* attribute), 30
 PeriodicEvalCallback (class in *dicee.callbacks*), 27
 Perturb (class in *dicee.callbacks*), 27
 polars_dataframe_indexer() (in module *dicee.read_preprocess_save_load_kg.util*), 151
 poly_NN() (*dicee.LFMult* method), 189
 poly_NN() (*dicee.models.function_space.LFMult* method), 81
 poly_NN() (*dicee.models.LFMult* method), 145
 polynomial() (*dicee.LFMult* method), 190
 polynomial() (*dicee.models.function_space.LFMult* method), 81
 polynomial() (*dicee.models.LFMult* method), 145
 pop() (*dicee.LFMult* method), 190
 pop() (*dicee.models.function_space.LFMult* method), 81
 pop() (*dicee.models.LFMult* method), 145
 pq (*dicee.analyse_experiments.Experiment* attribute), 20
 predict() (*dicee.KGE* method), 200
 predict() (*dicee.knowledge_graph_embeddings.KGE* method), 54
 predict_dataloader() (*dicee.models.base_model.BaseKGELightning* method), 61
 predict_dataloader() (*dicee.models.BaseKGELightning* method), 104
 predict_literals() (*dicee.KGE* method), 202
 predict_literals() (*dicee.knowledge_graph_embeddings.KGE* method), 56
 predict_missing_head_entity() (*dicee.KGE* method), 199
 predict_missing_head_entity() (*dicee.knowledge_graph_embeddings.KGE* method), 53
 predict_missing_relations() (*dicee.KGE* method), 200
 predict_missing_relations() (*dicee.knowledge_graph_embeddings.KGE* method), 53
 predict_missing_tail_entity() (*dicee.KGE* method), 200
 predict_missing_tail_entity() (*dicee.knowledge_graph_embeddings.KGE* method), 54
 predict_topk() (*dicee.KGE* method), 201
 predict_topk() (*dicee.knowledge_graph_embeddings.KGE* method), 54
 prepare_data() (*dicee.CVDataModule* method), 214
 prepare_data() (*dicee.dataset_classes.CVDataModule* method), 43
 preprocess_with_byte_pair_encoding() (*dicee.read_preprocess_save_load_kg.PreprocessKG* method), 153
 preprocess_with_byte_pair_encoding() (*dicee.read_preprocess_save_load_kg.preprocess.PreprocessKG* method), 148
 preprocess_with_byte_pair_encoding_with_padding() (*dicee.read_preprocess_save_load_kg.PreprocessKG* method), 153
 preprocess_with_byte_pair_encoding_with_padding() (*dicee.read_preprocess_save_load_kg.preprocess.PreprocessKG* method), 148

preprocess_with_pandas () (*dicee.read_preprocess_save_load_kg.PreprocessKG method*), 153
 preprocess_with_pandas () (*dicee.read_preprocess_save_load_kg.preprocess.PreprocessKG method*), 148
 preprocess_with_polars () (*dicee.read_preprocess_save_load_kg.PreprocessKG method*), 154
 preprocess_with_polars () (*dicee.read_preprocess_save_load_kg.preprocess.PreprocessKG method*), 149
 preprocesses_input_args () (*in module dicee.static_funcs*), 162
 PreprocessKG (*class in dicee.read_preprocess_save_load_kg*), 153
 PreprocessKG (*class in dicee.read_preprocess_save_load_kg.preprocess*), 148
 PrintCallback (*class in dicee.callbacks*), 21
 process (*dicee.trainer.torch_trainer.TorchTrainer attribute*), 166
 PseudoLabellingCallback (*class in dicee.callbacks*), 24
 Pyke (*class in dicee*), 172
 Pyke (*class in dicee.models*), 113
 Pyke (*class in dicee.models.real*), 91
 pykeen_model_kwarg (*dicee.config.Namespace attribute*), 31
 PykeenKGE (*class in dicee*), 190
 PykeenKGE (*class in dicee.models*), 139
 PykeenKGE (*class in dicee.models.pykeen_models*), 86

Q

q (*dicee.config.Namespace attribute*), 31
 q (*dicee.DeCaL attribute*), 177
 q (*dicee.Keci attribute*), 174
 q (*dicee.models.clifford.DeCaL attribute*), 71
 q (*dicee.models.clifford.Keci attribute*), 68
 q (*dicee.models.DeCaL attribute*), 134
 q (*dicee.models.Keci attribute*), 130
 qdrant_client (*dicee.scripts.index_serve.NeuralSearcher attribute*), 156
 QMult (*class in dicee*), 186
 QMult (*class in dicee.models*), 121
 QMult (*class in dicee.models.quaternion*), 88
 quaternion_mul () (*in module dicee.models*), 118
 quaternion_mul () (*in module dicee.models.static_funcs*), 92
 quaternion_mul_with_unit_norm () (*in module dicee.models*), 121
 quaternion_mul_with_unit_norm () (*in module dicee.models.quaternion*), 88
 quaternion_multiplication_followed_by_inner_product () (*dicee.models.QMult method*), 122
 quaternion_multiplication_followed_by_inner_product () (*dicee.models.quaternion.QMult method*), 88
 quaternion_multiplication_followed_by_inner_product () (*dicee.QMult method*), 187
 quaternion_normalizer () (*dicee.models.QMult static method*), 122
 quaternion_normalizer () (*dicee.models.quaternion.QMult static method*), 88
 quaternion_normalizer () (*dicee.QMult static method*), 187
 queries (*dicee.scripts.index_serve.StringListRequest attribute*), 157
 query_name_to_struct (*dicee.query_generator.QueryGenerator attribute*), 147
 query_name_to_struct (*dicee.QueryGenerator attribute*), 217
 QueryGenerator (*class in dicee*), 217
 QueryGenerator (*class in dicee.query_generator*), 147

R

r (*dicee.DeCaL attribute*), 177
 r (*dicee.Keci attribute*), 174
 r (*dicee.models.clifford.DeCaL attribute*), 71
 r (*dicee.models.clifford.Keci attribute*), 68
 r (*dicee.models.DeCaL attribute*), 134
 r (*dicee.models.Keci attribute*), 130
 random_prediction () (*in module dicee*), 197
 random_prediction () (*in module dicee.static_funcs*), 160
 random_seed (*dicee.config.Namespace attribute*), 31
 ratio (*dicee.callbacks.Perturb attribute*), 27
 re (*dicee.DeCaL attribute*), 177
 re (*dicee.models.clifford.DeCaL attribute*), 71
 re (*dicee.models.DeCaL attribute*), 134
 re_vocab (*dicee.evaluator.Evaluator attribute*), 48
 read_from_disk () (*in module dicee.read_preprocess_save_load_kg.util*), 152
 read_from_triple_store () (*in module dicee.read_preprocess_save_load_kg.util*), 152
 read_only_few (*dicee.config.Namespace attribute*), 31
 read_only_few (*dicee.knowledge_graph.KG attribute*), 52
 read_or_load_kg () (*in module dicee*), 197
 read_or_load_kg () (*in module dicee.static_funcs*), 160

read_with_pandas() (*in module dicee.read_preprocess_save_load_kg.util*), 152
read_with_polars() (*in module dicee.read_preprocess_save_load_kg.util*), 152
ReadFromDisk (*class in dicee.read_preprocess_save_load_kg*), 154
ReadFromDisk (*class in dicee.read_preprocess_save_load_kg.read_from_disk*), 149
reducer (*dicee.scripts.index_serve.StringListRequest attribute*), 157
rel2id (*dicee.query_generator.QueryGenerator attribute*), 147
rel2id (*dicee.QueryGenerator attribute*), 217
relation_embeddings (*dicee.AConvQ attribute*), 183
relation_embeddings (*dicee.ConvQ attribute*), 184
relation_embeddings (*dicee.DeCaL attribute*), 177
relation_embeddings (*dicee.DualE attribute*), 180
relation_embeddings (*dicee.LFMult attribute*), 189
relation_embeddings (*dicee.models.AConvQ attribute*), 123
relation_embeddings (*dicee.models.clifford.DeCaL attribute*), 71
relation_embeddings (*dicee.models.ConvQ attribute*), 123
relation_embeddings (*dicee.models.DeCaL attribute*), 134
relation_embeddings (*dicee.models.DualE attribute*), 146
relation_embeddings (*dicee.models.dualE.DualE attribute*), 77
relation_embeddings (*dicee.models.FMult attribute*), 142
relation_embeddings (*dicee.models.FMult2 attribute*), 144
relation_embeddings (*dicee.models.function_space.FMult attribute*), 78
relation_embeddings (*dicee.models.function_space.FMult2 attribute*), 80
relation_embeddings (*dicee.models.function_space.GFMult attribute*), 79
relation_embeddings (*dicee.models.function_space.LFMult attribute*), 80
relation_embeddings (*dicee.models.function_space.LFMultI attribute*), 80
relation_embeddings (*dicee.models.GFMult attribute*), 143
relation_embeddings (*dicee.models.LFMult attribute*), 144
relation_embeddings (*dicee.models.LFMultI attribute*), 144
relation_embeddings (*dicee.models.pykeen_models.PykeenKGE attribute*), 87
relation_embeddings (*dicee.models.PykeenKGE attribute*), 139
relation_embeddings (*dicee.models.quaternion.AConvQ attribute*), 90
relation_embeddings (*dicee.models.quaternion.ConvQ attribute*), 89
relation_embeddings (*dicee.PykeenKGE attribute*), 190
relation_to_idx (*dicee.knowledge_graph.KG attribute*), 52
relations_str (*dicee.knowledge_graph.KG property*), 52
reload_dataset() (*in module dicee*), 204
reload_dataset() (*in module dicee.dataset_classes*), 33
report (*dicee.DICE_Trainer attribute*), 198
report (*dicee.evaluator.Evaluator attribute*), 48
report (*dicee.Execute attribute*), 203
report (*dicee.executer.Execute attribute*), 50
report (*dicee.trainer.DICE_Trainer attribute*), 168
report (*dicee.trainer.dice_trainer.DICE_Trainer attribute*), 163
reports (*dicee.callbacks.Eval attribute*), 25
reports (*dicee.callbacks.PeriodicEvalCallback attribute*), 27
requires_grad_for_interactions (*dicee.CKeci attribute*), 173
requires_grad_for_interactions (*dicee.Keci attribute*), 174
requires_grad_for_interactions (*dicee.models.CKeci attribute*), 133
requires_grad_for_interactions (*dicee.models.clifford.CKeci attribute*), 70
requires_grad_for_interactions (*dicee.models.clifford.Keci attribute*), 68
requires_grad_for_interactions (*dicee.models.Keci attribute*), 131
resid_dropout (*dicee.models.transformers.CausalSelfAttention attribute*), 96
residual_convolution() (*dicee.AConEx method*), 182
residual_convolution() (*dicee.AConvO method*), 183
residual_convolution() (*dicee.AConvQ method*), 183
residual_convolution() (*dicee.ConEx method*), 186
residual_convolution() (*dicee.ConvO method*), 185
residual_convolution() (*dicee.ConvQ method*), 184
residual_convolution() (*dicee.models.AConEx method*), 116
residual_convolution() (*dicee.models.AConvO method*), 130
residual_convolution() (*dicee.models.AConvQ method*), 124
residual_convolution() (*dicee.models.complex.AConEx method*), 75
residual_convolution() (*dicee.models.complex.ConEx method*), 74
residual_convolution() (*dicee.models.ConEx method*), 116
residual_convolution() (*dicee.models.ConvO method*), 129
residual_convolution() (*dicee.models.ConvQ method*), 123
residual_convolution() (*dicee.models.octonion.AConvO method*), 86
residual_convolution() (*dicee.models.octonion.ConvO method*), 85

```

residual_convolution() (dicee.models.quaternion.AConvQ method), 90
residual_convolution() (dicee.models.quaternion.ConvQ method), 90
retrieve_embedding() (dicee.scripts.index_serve.NeuralSearcher method), 156
retrieve_embeddings() (in module dicee.scripts.index_serve), 156
return_multi_hop_query_results() (dicee.KGE method), 201
return_multi_hop_query_results() (dicee.knowledge_graph_embeddings.KGE method), 55
root() (in module dicee.scripts.index_serve), 156
roots (dicee.models.FMult attribute), 143
roots (dicee.models.function_space.FMult attribute), 79
roots (dicee.models.function_space.GFMult attribute), 79
roots (dicee.models.GFMult attribute), 143
runtime (dicee.analyse_experiments.Experiment attribute), 20

```

S

```

sample_counter (dicee.abstracts.AbstractPPECallback attribute), 17
sample_entity() (dicee.abstracts.BaseInteractiveKGE method), 15
sample_relation() (dicee.abstracts.BaseInteractiveKGE method), 15
sample_triples_ratio (dicee.config.Namespace attribute), 31
sample_triples_ratio (dicee.knowledge_graph.KG attribute), 52
sampling_ratio (dicee.dataset_classes.LiteralDataset attribute), 45
sampling_ratio (dicee.LiteralDataset attribute), 215, 216
sanity_check_callback_args() (in module dicee.sanity_checkers), 155
sanity_checking_with_arguments() (in module dicee.sanity_checkers), 155
save() (dicee.abstracts.BaseInteractiveKGE method), 15
save() (dicee.read_preprocess_save_load_kg.LoadSaveToDisk method), 154
save() (dicee.read_preprocess_save_load_kg.save_load_disk.LoadSaveToDisk method), 150
save_checkpoint() (dicee.abstracts.AbstractTrainer static method), 14
save_checkpoint_model() (in module dicee), 197
save_checkpoint_model() (in module dicee.static_funcs), 160
save_embeddings() (in module dicee), 197
save_embeddings() (in module dicee.static_funcs), 160
save_embeddings_as_csv (dicee.config.Namespace attribute), 29
save_every_n_epochs (dicee.config.Namespace attribute), 32
save_experiment() (dicee.analyse_experiments.Experiment method), 20
save_model_at_every_epoch (dicee.config.Namespace attribute), 31
save_model_every_n_epoch (dicee.callbacks.PeriodicEvalCallback attribute), 27
save_numpy_ndarray() (in module dicee), 196
save_numpy_ndarray() (in module dicee.read_preprocess_save_load_kg.util), 153
save_numpy_ndarray() (in module dicee.static_funcs), 160
save_pickle() (in module dicee), 196
save_pickle() (in module dicee.read_preprocess_save_load_kg.util), 153
save_pickle() (in module dicee.static_funcs), 160
save_queries() (dicee.query_generator.QueryGenerator method), 148
save_queries() (dicee.QueryGenerator method), 218
save_queries_and_answers() (dicee.query_generator.QueryGenerator static method), 148
save_queries_and_answers() (dicee.QueryGenerator static method), 218
save_trained_model() (dicee.Execute method), 203
save_trained_model() (dicee.executer.Execute method), 50
scalar_batch_NN() (dicee.LFMult method), 189
scalar_batch_NN() (dicee.models.function_space.LFMult method), 81
scalar_batch_NN() (dicee.models.LFMult method), 145
scaler (dicee.callbacks.Perturb attribute), 27
scaler (dicee.trainer.torch_trainer_ddp.NodeTrainer attribute), 168
scheduler (dicee.callbacks.LRScheduler attribute), 28
score() (dicee.ComplEx static method), 182
score() (dicee.DistMult method), 173
score() (dicee.Keci method), 176
score() (dicee.models.clifford.Keci method), 70
score() (dicee.models.ComplEx static method), 117
score() (dicee.models.complex.ComplEx static method), 76
score() (dicee.models.DistMult method), 112
score() (dicee.models.Keci method), 133
score() (dicee.models.octonion.OMult method), 84
score() (dicee.models.OMult method), 128
score() (dicee.models.QMult method), 122
score() (dicee.models.quaternion.QMult method), 89
score() (dicee.models.real.DistMult method), 91

```

```

score() (dicee.models.real.TransE method), 91
score() (dicee.models.TransE method), 113
score() (dicee.OMult method), 188
score() (dicee.QMult method), 187
score() (dicee.TransE method), 176
score_func(dicee.models.FMult2 attribute), 143
score_func(dicee.models.function_space.FMult2 attribute), 79
scoring_technique(dicee.analyse_experiments.Experiment attribute), 20
scoring_technique(dicee.config.Namespace attribute), 30
search() (dicee.scripts.index_serve.NeuralSearcher method), 156
search_embeddings() (in module dicee.scripts.index_serve), 156
search_embeddings_batch() (in module dicee.scripts.index_serve), 158
seed(dicee.query_generator.QueryGenerator attribute), 147
seed(dicee.QueryGenerator attribute), 217
select_model() (in module dicee), 196
select_model() (in module dicee.static_funcs), 160
selected_optimizer(dicee.BaseKGE attribute), 194
selected_optimizer(dicee.models.base_model.BaseKGE attribute), 65
selected_optimizer(dicee.models.BaseKGE attribute), 107, 111, 114, 119, 125, 138, 141
separator(dicee.config.Namespace attribute), 30
separator(dicee.knowledge_graph.KG attribute), 52
sequential_vocabulary_construction() (dicee.read_preprocess_save_load_kg.PreprocessKG method), 154
sequential_vocabulary_construction() (dicee.read_preprocess_save_load_kg.preprocess.PreprocessKG method), 149
serve() (in module dicee.scripts.index_serve), 158
set_global_seed() (dicee.query_generator.QueryGenerator method), 147
set_global_seed() (dicee.QueryGenerator method), 217
set_model_eval_mode() (dicee.abstracts.BaseInteractiveKGE method), 15
set_model_train_mode() (dicee.abstracts.BaseInteractiveKGE method), 14
setup() (dicee.CVDataModule method), 213
setup() (dicee.dataset_classes.CVDataModule method), 42
setup_executor() (dicee.Execute method), 203
setup_executor() (dicee.executer.Execute method), 50
Shallom(class in dicee), 188
Shallom(class in dicee.models), 113
Shallom(class in dicee.models.real), 91
shallom(dicee.models.real.Shallom attribute), 91
shallom(dicee.models.Shallom attribute), 113
shallom(dicee.Shallom attribute), 188
single_hop_query_answering() (dicee.KGE method), 201
single_hop_query_answering() (dicee.knowledge_graph_embeddings.KGE method), 55
snapshot_dir(dicee.callbacks.LRScheduler attribute), 28
snapshot_loss(dicee.callbacks.LRScheduler attribute), 28
sparql_endpoint(dicee.config.Namespace attribute), 30
sparql_endpoint(dicee.knowledge_graph.KG attribute), 51
start() (dicee.DICE_Trainer method), 198
start() (dicee.Execute method), 204
start() (dicee.executer.Execute method), 50
start() (dicee.read_preprocess_save_load_kg.PreprocessKG method), 153
start() (dicee.read_preprocess_save_load_kg.preprocess.PreprocessKG method), 148
start() (dicee.read_preprocess_save_load_kg.read_from_disk.ReadFromDisk method), 149
start() (dicee.read_preprocess_save_load_kg.ReadFromDisk method), 154
start() (dicee.trainer.DICE_Trainer method), 169
start() (dicee.trainer.dice_trainer.DICE_Trainer method), 164
start_time(dicee.callbacks.PrintCallback attribute), 22
start_time(dicee.Execute attribute), 203
start_time(dicee.executer.Execute attribute), 50
step() (dicee.EnsembleKGE method), 196
step() (dicee.models.ADOPT method), 100
step() (dicee.models.adopt.ADOPT method), 57
step() (dicee.models.ensemble.EnsembleKGE method), 78
step_count(dicee.callbacks.LRScheduler attribute), 28
storage_path(dicee.config.Namespace attribute), 29
storage_path(dicee.DICE_Trainer attribute), 198
storage_path(dicee.trainer.DICE_Trainer attribute), 168
storage_path(dicee.trainer.dice_trainer.DICE_Trainer attribute), 164
store() (in module dicee), 197
store() (in module dicee.static_funcs), 160
store_ensemble() (dicee.abstracts.AbstractPPECallback method), 18

```

strategy (*dicee.abstracts.AbstractTrainer* attribute), 13
StringListRequest (class in *dicee.scripts.index_serve*), 156
 SWA (class in *dicee.callbacks*), 28
 swa (*dicee.config.Namespace* attribute), 32
 swa_c_epochs (*dicee.callbacks.SWA* attribute), 29
 swa_lr (*dicee.callbacks.SWA* attribute), 29
 swa_model (*dicee.callbacks.SWA* attribute), 29
 swa_n (*dicee.callbacks.SWA* attribute), 29
 swa_start_epoch (*dicee.callbacks.SWA* attribute), 29
 swa_start_epoch (*dicee.config.Namespace* attribute), 32

T

T () (*dicee.DualE* method), 181
 T () (*dicee.models.DualE* method), 146
 T () (*dicee.models.dualE.DualE* method), 77
 t_cnorm () (*dicee.abstracts.InteractiveQueryDecomposition* method), 16
 t_norm () (*dicee.abstracts.InteractiveQueryDecomposition* method), 16
 target_dim (*dicee.AllvsAll* attribute), 208
 target_dim (*dicee.dataset_classes.AllvsAll* attribute), 37
 target_dim (*dicee.dataset_classes.MultiLabelDataset* attribute), 34
 target_dim (*dicee.dataset_classes.OnevsAllDataset* attribute), 35
 target_dim (*dicee.knowledge_graph.KG* attribute), 52
 target_dim (*dicee.MultiLabelDataset* attribute), 205
 target_dim (*dicee.OnevsAllDataset* attribute), 206
 temperature (*dicee.BytE* attribute), 192
 temperature (*dicee.models.transformers.BytE* attribute), 93
 tensor_t_norm () (*dicee.abstracts.InteractiveQueryDecomposition* method), 16
 TensorParallel (class in *dicee.trainer.model_parallelism*), 165
 test_dataloader () (*dicee.models.base_model.BaseKGELightning* method), 60
 test_dataloader () (*dicee.models.BaseKGELightning* method), 103
 test_epoch_end () (*dicee.models.base_model.BaseKGELightning* method), 60
 test_epoch_end () (*dicee.models.BaseKGELightning* method), 103
 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), 147
 test_path (*dicee.QueryGenerator* attribute), 217
 timeit () (in module *dicee*), 196, 204
 timeit () (in module *dicee.read_preprocess_save_load_kg.util*), 152
 timeit () (in module *dicee.static_funcs*), 160
 timeit () (in module *dicee.static_preprocess_funcs*), 162
 to () (*dicee.EnsembleKGE* method), 196
 to () (*dicee.KGE* method), 199
 to () (*dicee.knowledge_graph_embeddings.KGE* method), 53
 to () (*dicee.models.ensemble.EnsembleKGE* method), 78
 to_df () (*dicee.analyse_experiments.Experiment* method), 20
 topk (*dicee.BytE* attribute), 192
 topk (*dicee.models.transformers.BytE* attribute), 93
 topk (*dicee.scripts.index_serve.NeuralSearcher* attribute), 156
 torch_ordered_shaped_bpe_entities (*dicee.dataset_classes.MultiLabelDataset* attribute), 34
 torch_ordered_shaped_bpe_entities (*dicee.MultiLabelDataset* attribute), 205
 TorchDDPTrainer (class in *dicee.trainer.torch_trainer_ddp*), 167
 TorchTrainer (class in *dicee.trainer.torch_trainer*), 166
 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), 168
 train_data (*dicee.AllvsAll* attribute), 207
 train_data (*dicee.dataset_classes.AllvsAll* attribute), 37
 train_data (*dicee.dataset_classes.KvsAll* attribute), 36
 train_data (*dicee.dataset_classes.KvsSampleDataset* attribute), 39
 train_data (*dicee.dataset_classes.MultiClassClassificationDataset* attribute), 35
 train_data (*dicee.dataset_classes.OnevsAllDataset* attribute), 35
 train_data (*dicee.dataset_classes.OnevsSample* attribute), 37, 38
 train_data (*dicee.KvsAll* attribute), 207
 train_data (*dicee.KvsSampleDataset* attribute), 210

train_data (*dicee.MultiClassClassificationDataset* attribute), 205
 train_data (*dicee.OnevsAllDataset* attribute), 206
 train_data (*dicee.OnevsSample* attribute), 208, 209
 train_dataloader() (*dicee.CVDataModule* method), 212
 train_dataloader() (*dicee.dataset_classes.CVDataModule* method), 41
 train_dataloader() (*dicee.models.base_model.BaseKGELightning* method), 61
 train_dataloader() (*dicee.models.BaseKGELightning* method), 104
 train_dataloaders (*dicee.trainer.torch_trainer.TorchTrainer* attribute), 166
 train_dataset_loader (*dicee.trainer.torch_trainer_ddp.NodeTrainer* attribute), 168
 train_file_path (*dicee.dataset_classes.LiteralDataset* attribute), 44, 45
 train_file_path (*dicee.LiteralDataset* attribute), 215, 216
 train_h1 (*dicee.analyse_experiments.Experiment* attribute), 20
 train_h3 (*dicee.analyse_experiments.Experiment* attribute), 20
 train_h10 (*dicee.analyse_experiments.Experiment* attribute), 20
 train_indices_target (*dicee.dataset_classes.MultiLabelDataset* attribute), 34
 train_indices_target (*dicee.MultiLabelDataset* attribute), 205
 train_k_vs_all() (*dicee.abstracts.BaseInteractiveTrainKGE* method), 18
 train_literals() (*dicee.abstracts.BaseInteractiveTrainKGE* method), 18
 train_mode (*dicee.EnsembleKGE* attribute), 195
 train_mode (*dicee.models.ensemble.EnsembleKGE* attribute), 78
 train_mrr (*dicee.analyse_experiments.Experiment* attribute), 20
 train_path (*dicee.query_generator.QueryGenerator* attribute), 147
 train_path (*dicee.QueryGenerator* attribute), 217
 train_set (*dicee.BPE_NegativeSamplingDataset* attribute), 204
 train_set (*dicee.dataset_classes.BPE_NegativeSamplingDataset* attribute), 34
 train_set (*dicee.dataset_classes.MultiLabelDataset* attribute), 34
 train_set (*dicee.dataset_classes.NegSampleDataset* attribute), 40
 train_set (*dicee.dataset_classes.TriplePredictionDataset* attribute), 41
 train_set (*dicee.MultiLabelDataset* attribute), 205
 train_set (*dicee.NegSampleDataset* attribute), 210
 train_set (*dicee.TriplePredictionDataset* attribute), 211
 train_set_idx (*dicee.CVDataModule* attribute), 212
 train_set_idx (*dicee.dataset_classes.CVDataModule* attribute), 41
 train_set_target (*dicee.knowledge_graph.KG* attribute), 52
 train_target (*dicee.AllvsAll* attribute), 207
 train_target (*dicee.dataset_classes.AllvsAll* attribute), 37
 train_target (*dicee.dataset_classes.KvsAll* attribute), 36
 train_target (*dicee.dataset_classes.KvsSampleDataset* attribute), 39
 train_target (*dicee.KvsAll* attribute), 207
 train_target (*dicee.KvsSampleDataset* attribute), 210
 train_target_indices (*dicee.knowledge_graph.KG* attribute), 52
 train_triples() (*dicee.abstracts.BaseInteractiveTrainKGE* method), 18
 trained_model (*dicee.Execute* attribute), 203
 trained_model (*dicee.executer.Execute* attribute), 50
 trainer (*dicee.config.Namespace* attribute), 30
 trainer (*dicee.DICE_Trainer* attribute), 198
 trainer (*dicee.Execute* attribute), 203
 trainer (*dicee.executer.Execute* attribute), 50
 trainer (*dicee.trainer.DICE_Trainer* attribute), 168
 trainer (*dicee.trainer.dice_trainer.DICE_Trainer* attribute), 163
 trainer (*dicee.trainer.torch_trainer_ddp.NodeTrainer* attribute), 167
 training_step (*dicee.trainer.torch_trainer.TorchTrainer* attribute), 166
 training_step() (*dicee.BytE* method), 192
 training_step() (*dicee.models.base_model.BaseKGELightning* method), 58
 training_step() (*dicee.models.BaseKGELightning* method), 101
 training_step() (*dicee.models.transformers.BytE* method), 94
 training_step_outputs (*dicee.models.base_model.BaseKGELightning* attribute), 58
 training_step_outputs (*dicee.models.BaseKGELightning* attribute), 101
 training_technique (*dicee.knowledge_graph.KG* attribute), 52
 TransE (*class in dicee*), 176
 TransE (*class in dicee.models*), 112
 TransE (*class in dicee.models.real*), 91
 transfer_batch_to_device() (*dicee.CVDataModule* method), 213
 transfer_batch_to_device() (*dicee.dataset_classes.CVDataModule* method), 42
 transformer (*dicee.BytE* attribute), 192
 transformer (*dicee.models.transformers.BytE* attribute), 93
 transformer (*dicee.models.transformers.GPT* attribute), 98
 trapezoid() (*dicee.models.FMult2* method), 144

`trapezoid()` (*dicee.models.function_space.FMult2 method*), 80
`tri_score()` (*dicee.LFMult method*), 189
`tri_score()` (*dicee.models.function_space.LFMult method*), 81
`tri_score()` (*dicee.models.function_space.LFMult1 method*), 80
`tri_score()` (*dicee.models.LFMult method*), 145
`tri_score()` (*dicee.models.LFMult1 method*), 144
`triple_score()` (*dicee.KGE method*), 201
`triple_score()` (*dicee.knowledge_graph_embeddings.KGE method*), 54
`TriplePredictionDataset` (*class in dicee*), 211
`TriplePredictionDataset` (*class in dicee.dataset_classes*), 40
`tuple2list()` (*dicee.query_generator.QueryGenerator method*), 147
`tuple2list()` (*dicee.QueryGenerator method*), 217

U

`unlabelled_size` (*dicee.callbacks.PseudoLabellingCallback attribute*), 24
`unmap()` (*dicee.query_generator.QueryGenerator method*), 147
`unmap()` (*dicee.QueryGenerator method*), 218
`unmap_query()` (*dicee.query_generator.QueryGenerator method*), 147
`unmap_query()` (*dicee.QueryGenerator method*), 218

V

`val_aswa` (*dicee.callbacks.ASWA attribute*), 24
`val_dataloader()` (*dicee.models.base_model.BaseKGELightning method*), 61
`val_dataloader()` (*dicee.models.BaseKGELightning method*), 103
`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*), 147
`val_path` (*dicee.QueryGenerator attribute*), 217
`validate_knowledge_graph()` (*in module dicee.sanity_checkers*), 155
`vocab_preparation()` (*dicee.evaluator.Evaluator method*), 48
`vocab_size` (*dicee.models.transformers.GPTConfig attribute*), 97
`vocab_to_parquet()` (*in module dicee*), 197
`vocab_to_parquet()` (*in module dicee.static_funcs*), 161
`vtp_score()` (*dicee.LFMult method*), 189
`vtp_score()` (*dicee.models.function_space.LFMult method*), 81
`vtp_score()` (*dicee.models.function_space.LFMult1 method*), 80
`vtp_score()` (*dicee.models.LFMult method*), 145
`vtp_score()` (*dicee.models.LFMult1 method*), 144

W

`warmup_steps` (*dicee.callbacks.LRScheduler attribute*), 28
`weight` (*dicee.models.transformers.LayerNorm attribute*), 95
`weight_decay` (*dicee.BaseKGE attribute*), 194
`weight_decay` (*dicee.config.Namespace attribute*), 30
`weight_decay` (*dicee.models.base_model.BaseKGE attribute*), 64
`weight_decay` (*dicee.models.BaseKGE attribute*), 107, 111, 114, 119, 125, 138, 141
`weights` (*dicee.models.FMult attribute*), 143
`weights` (*dicee.models.function_space.FMult attribute*), 79
`weights` (*dicee.models.function_space.GFMult attribute*), 79
`weights` (*dicee.models.GFMult attribute*), 143
`write_csv_from_model_parallel()` (*in module dicee*), 197
`write_csv_from_model_parallel()` (*in module dicee.static_funcs*), 161
`write_links()` (*dicee.query_generator.QueryGenerator method*), 147
`write_links()` (*dicee.QueryGenerator method*), 217
`write_report()` (*dicee.Execute method*), 203
`write_report()` (*dicee.executer.Execute method*), 50

X

`x_values` (*dicee.LFMult attribute*), 189
`x_values` (*dicee.models.function_space.LFMult attribute*), 80
`x_values` (*dicee.models.LFMult attribute*), 144