AmpliGraph

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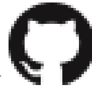
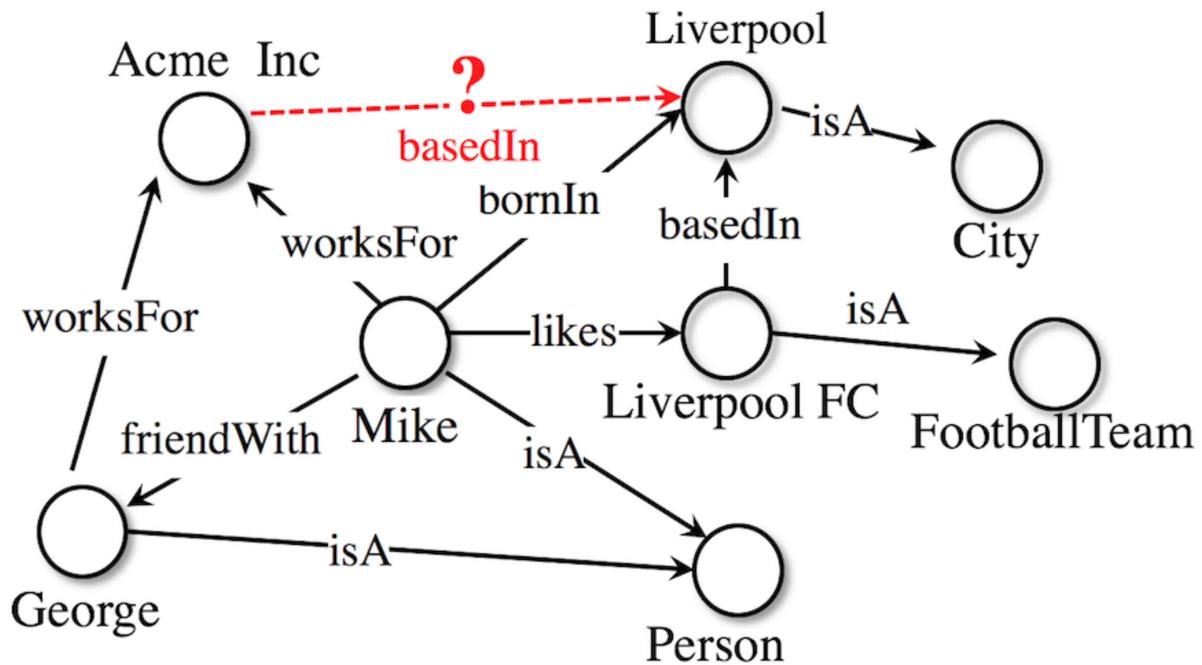
Open source Python library that predicts links between concepts in a knowledge graph.

View the GitHub repository 

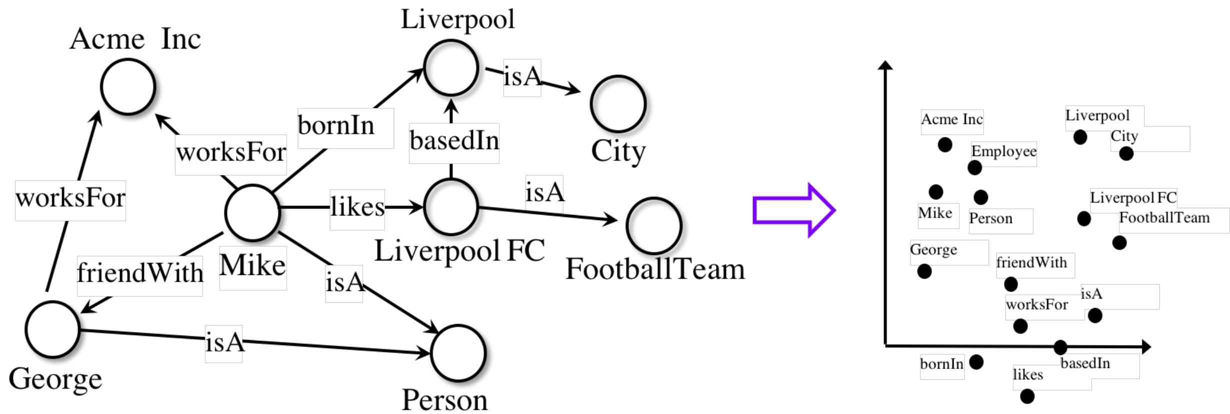
AmpliGraph is a suite of neural machine learning models for relational Learning, a branch of machine learning that deals with supervised learning on knowledge graphs.



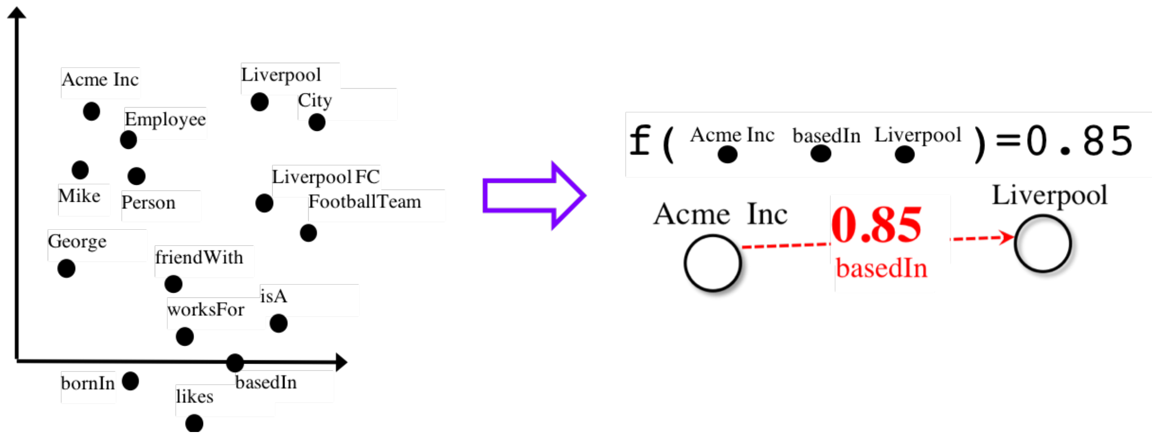
Use AmpliGraph if you need to:

- Discover new knowledge from an existing knowledge graph.
- Complete large knowledge graphs with missing statements.
- Generate stand-alone knowledge graph embeddings.
- Develop and evaluate a new relational model.

AmpliGraph's machine learning models generate **knowledge graph embeddings**, vector representations of concepts in a metric space:



It then combines embeddings with model-specific scoring functions to predict unseen and novel links:



CHAPTER 1

Key Features

- **Intuitive APIs**: AmpliGraph APIs are designed to reduce the code amount required to learn models that predict links in knowledge graphs.
- **GPU-Ready**: AmpliGraph is based on TensorFlow, and it is designed to run seamlessly on CPU and GPU devices - to speed-up training.
- **Extensible**: Roll your own knowledge graph embeddings model by extending AmpliGraph base estimators.

CHAPTER 2

Modules

AmpliGraph includes the following submodules:

- **Input**: Helper functions to load datasets (knowledge graphs).
- **Latent Feature Models**: knowledge graph embedding models. AmpliGraph contains: TransE, DistMult, ComplEx, HolE. (More to come!)
- **Evaluation**: Metrics and evaluation protocols to assess the predictive power of the models.

CHAPTER 3

How to Cite

If you like AmpliGraph and you use it in your project, why not starring the project on GitHub!

If you instead use AmpliGraph in an academic publication, cite as:

```
@misc{ampligraph,
  author= {Luca Costabello and
           Sumit Pai and
           Chan Le Van and
           Rory McGrath and
           Nick McCarthy},
  title = {{AmpliGraph: a Library for Representation Learning on Knowledge Graphs}},
  month = mar,
  year  = 2019,
  doi   = {10.5281/zenodo.2595043},
  url   = {https://doi.org/10.5281/zenodo.2595043}
}
```

3.1 Installation

3.1.1 Prerequisites

- Linux Box
- Python 3.6

Provision a Virtual Environment

Create and activate a virtual environment (conda)

```
conda create --name ampligraph python=3.6
source activate ampligraph
```

Install TensorFlow

AmpliGraph is built on TensorFlow 1.x. Install from pip or conda:

CPU-only

```
pip install tensorflow==1.12.0

or

conda install tensorflow=1.12.0
```

GPU support

```
pip install tensorflow-gpu==1.12.0

or

conda install tensorflow-gpu=1.12.0
```

3.1.2 Install AmpliGraph

Install the latest stable release from pip:

```
pip install ampligraph
```

If instead you want the most recent development version, you can clone the repository and install from source as: See the *How to Contribute guide* for details.

```
git clone https://github.com/Accenture/AmpliGraph.git
git checkout develop
cd AmpliGraph
pip install -e .
```

3.1.3 Sanity Check

```
>> import ampligraph
>> ampligraph.__version__
'1.0.2'
```

3.2 Background

Knowledge graphs are graph-based knowledge bases whose facts are modeled as relationships between entities. Knowledge graph research led to broad-scope graphs such as DBpedia [ABK+07], WordNet [Pri10], and YAGO [SKW07]. Countless domain-specific knowledge graphs have also been published on the web, giving birth to the so-called Web of Data [BHBL11].

Formally, a knowledge graph $\mathcal{G} = \{(sub, pred, obj)\} \subseteq \mathcal{E} \times \mathcal{R} \times \mathcal{E}$ is a set of $(sub, pred, obj)$ triples, each including a subject $sub \in \mathcal{E}$, a predicate $pred \in \mathcal{R}$, and an object $obj \in \mathcal{E}$. $\mathcal{E}$ and $\mathcal{R}$ are the sets of all entities and relation types of $\mathcal{G}$.

Knowledge graph embedding models are neural architectures that encode concepts from a knowledge graph (i.e. entities $\mathcal{E}$ and relation types $\mathcal{R}$) into low-dimensional, continuous vectors $\in \mathcal{R}^k$. Such textit{knowledge graph embeddings} have applications in knowledge graph completion, entity resolution, and link-based clustering, just to cite a few [NMTG16]. Knowledge graph embeddings are learned by training a neural architecture over a graph. Although such architectures vary, the training phase always consists in minimizing a loss function $\mathcal{L}$ that includes a *scoring function* $f_m(t)$, i.e. a model-specific function that assigns a score to a triple $t = (sub, pred, obj)$.

The goal of the optimization procedure is learning optimal embeddings, such that the scoring function is able to assign high scores to positive statements and low scores to statements unlikely to be true. Existing models propose scoring functions that combine the embeddings $\mathbf{e}_{sub}, \mathbf{e}_{pred}, \mathbf{e}_{obj} \in \mathcal{R}^k$ of the subject, predicate, and object of triple $t = (sub, pred, obj)$ using different intuitions: TransE [BUGD+13] relies on distances, DistMult [YYH+14] and ComplEx [TWR+16] are bilinear-diagonal models, HolE [NRP+16] uses circular correlation. While the above models can be interpreted as multilayer perceptrons, others such as ConvE include convolutional layers [DMSR18].

As example, the scoring function of TransE computes a similarity between the embedding of the subject $\mathbf{e}_{sub}$ translated by the embedding of the predicate $\mathbf{e}_{pred}$ and the embedding of the object $\mathbf{e}_{obj}$, using the L_1 or L_2 norm $||\cdot||$:

$$f_{TransE} = -||\mathbf{e}_{sub} + \mathbf{e}_{pred} - \mathbf{e}_{obj}||_n$$

Such scoring function is then used on positive and negative triples t^+, t^- in the loss function. This can be for example a pairwise margin-based loss, as shown in the equation below:

$$\mathcal{L}(\Theta) = \sum_{t^+ \in \mathcal{G}} \sum_{t^- \in \mathcal{N}} max(0, [\gamma + f_m(t^-; \Theta) - f_m(t^+; \Theta)])$$

where Θ are the embeddings learned by the model, f_m is the model-specific scoring function, $\gamma \in \mathcal{R}$ is the margin and $\mathcal{N}$ is a set of negative triples generated with a corruption heuristic [BUGD+13].

3.3 API

AmpliGraph includes the following submodules:

3.3.1 Datasets

Helper functions to load knowledge graphs.

Note: It is recommended to set the `AMPLIGRAPH_DATA_HOME` environment variable:

```
export AMPLIGRAPH_DATA_HOME=/YOUR/PATH/TO/datasets
```

When attempting to load a dataset, the module will first check if `AMPLIGRAPH_DATA_HOME` is set. If it is, it will search this location for the required dataset. If the dataset is not found it will be downloaded and placed in this directory.

If `AMPLIGRAPH_DATA_HOME` has not been set the databases will be saved in the following directory:

```
~/ampligraph_datasets
```

Dataset-Specific Loaders

Use these helpers functions to load datasets used in graph representation learning literature. The functions will **automatically download** the datasets if they are not present in `~/ampligraph_datasets` or at the location set in `AMPLIGRAPH_DATA_HOME`.

load_wn18([check_md5hash])	Load the WN18 dataset
load_fb15k([check_md5hash])	Load the FB15k dataset
load_fb15k_237([check_md5hash, clean_unseen])	Load the FB15k-237 dataset
load_yago3_10([check_md5hash, clean_unseen])	Load the YAGO3-10 dataset
load_wn18rr([check_md5hash, clean_unseen])	Load the WN18RR dataset

load_wn18

`ampligraph.datasets.`**`load_wn18`**(*check_md5hash=False*)

Load the WN18 dataset

WN18 is a subset of Wordnet. It was first presented by [BUGD+13].

The WN18 dataset is loaded from file if it exists at the `AMPLIGRAPH_DATA_HOME` location. IF `AMPLIGRAPH_DATA_HOME` is not set the the default `~/ampligraph_datasets` is checked.

If the dataset is not found at either location it is downloaded and placed in `AMPLIGRAPH_DATA_HOME` or `~/ampligraph_datasets`.

The dataset is divided in three splits:

- `train`: 141,442 triples
- `valid` 5,000 triples
- `test` 5,000 triples

Dataset	Train	Valid	Test	Entities	Relations
WN18	141,442	5,000	5,000	40,943	18

> **Warning:** The dataset includes a large number of inverse relations, and its use in experiments has been deprecated. Use WN18RR instead.

Returns **splits** – The dataset splits {'train': train, 'valid': valid, 'test': test}. Each split is an ndarray of shape [n, 3].

Return type dict

Examples

```
>>> from ampligraph.datasets import load_wn18
>>> X = load_wn18()
>>> X['test'][:3]
array([['06845599', '_member_of_domain_usage', '03754979'],
       ['00789448', '_verb_group', '01062739'],
       ['10217831', '_hyponym', '10682169']], dtype=object)
```

load_fb15k

`ampligraph.datasets.load_fb15k(check_md5hash=False)`

Load the FB15k dataset

FB15k is a split of Freebase, first proposed by [BUGD+13].

The FB15k dataset is loaded from file if it exists at the `AMPLIGRAPH_DATA_HOME` location. If `AMPLIGRAPH_DATA_HOME` is not set the the default `~/ampligraph_datasets` is checked.

If the dataset is not found at either location it is downloaded and placed in `AMPLIGRAPH_DATA_HOME` or `~/ampligraph_datasets`.

The dataset is divided in three splits:

- `train`
- `valid`
- `test`

Dataset	Train	Valid	Test	Entities	Relations
FB15K	483,142	50,000	59,071	14,951	1,345

Warning: The dataset includes a large number of inverse relations, and its use in experiments has been deprecated. Use FB15k-237 instead.

Returns splits – The dataset splits: {'train': train, 'valid': valid, 'test': test}. Each split is an ndarray of shape [n, 3].

Return type dict

Examples

```
>>> from ampligraph.datasets import load_fb15k
>>> X = load_fb15k()
>>> X['test'][:3]
array([['/m/01qscs',
        '/award/award_nominee/award_nominations./award/award_nomination/award',
        '/m/02x8n1n'],
       ['/m/040db', '/base/activism/activist/area_of_activism', '/m/0148d'],
       ['/m/08966',
        '/travel/travel_destination/climate./travel/travel_destination_monthly_
↪climate/month',
        '/m/05lf_']], dtype=object)
```

load_fb15k_237

`ampligraph.datasets.load_fb15k_237(check_md5hash=False, clean_unseen=True)`

Load the FB15k-237 dataset

FB15k-237 is a reduced version of FB15K. It was first proposed by [TCP+15].

The FB15k-237 dataset is loaded from file if it exists at the `AMPLIGRAPH_DATA_HOME` location. If `AMPLIGRAPH_DATA_HOME` is not set the the default `~/ampligraph_datasets` is checked.

If the dataset is not found at either location it is downloaded and placed in `AMPLIGRAPH_DATA_HOME` or `~/ampligraph_datasets`.

The dataset is divided in three splits:

- `train`
- `valid`
- `test`

Dataset	Train	Valid	Test	Entities	Relations
FB15K-237	272,115	17,535	20,466	14,541	237

> **Warning:** FB15K-237's validation set contains 8 unseen entities over 9 triples. The test set has 29 unseen entities, distributed over 28 triples.

Parameters **clean_unseen** (*bool*) – If `True`, filters triples in validation and test sets that include entities not present in the training set.

Returns **splits** – The dataset splits: {'train': train, 'valid': valid, 'test': test}. Each split is an ndarray of shape [n, 3].

Return type dict

Examples

```
>>> from ampligraph.datasets import load_fb15k_237
>>> X = load_fb15k_237()
>>> X["train"][2]
array(['/m/07s9rl0', '/media_common/netflix_genre/titles', '/m/0170z3'],
  dtype=object)
```

load_yago3_10

`ampligraph.datasets.`**`load_yago3_10`**(*check_md5hash=False*, *clean_unseen=True*)

Load the YAGO3-10 dataset

The dataset is a split of YAGO3 [MBS13], and has been first presented in [DMSR18].

The YAGO3-10 dataset is loaded from file if it exists at the `AMPLIGRAPH_DATA_HOME` location. If `AMPLIGRAPH_DATA_HOME` is not set the the default `~/ampligraph_datasets` is checked.

If the dataset is not found at either location it is downloaded and placed in `AMPLIGRAPH_DATA_HOME` or `~/ampligraph_datasets`.

It is divided in three splits:

- `train`
- `valid`
- `test`

Dataset	Train	Valid	Test	Entities	Relations
YAGO3-10	1,079,040	5,000	5,000	123,182	37

Returns splits – The dataset splits: {'train': train, 'valid': valid, 'test': test}. Each split is an ndarray of shape [n, 3].

Return type dict

Examples

```
>>> from ampligraph.datasets import load_yago3_10
>>> X = load_yago3_10()
>>> X["valid"][0]
array(['Mikheil_Khutsishvili', 'playsFor', 'FC_Merani_Tbilisi'], dtype=object)
```

load_wn18rr

`ampligraph.datasets.load_wn18rr(check_md5hash=False, clean_unseen=True)`

Load the WN18RR dataset

The dataset is described in [DMSR18].

The WN18RR dataset is loaded from file if it exists at the `AMPLIGRAPH_DATA_HOME` location. If `AMPLIGRAPH_DATA_HOME` is not set the the default `~/ampligraph_datasets` is checked.

If the dataset is not found at either location it is downloaded and placed in `AMPLIGRAPH_DATA_HOME` or `~/ampligraph_datasets`.

It is divided in three splits:

- `train`
- `valid`
- `test`

Dataset	Train	Valid	Test	Entities	Relations
WN18RR	86,835	3,034	3,134	40,943	11

> **Warning:** WN18RR's validation set contains 198 unseen entities over 210 triples. The test set has 209 unseen entities, distributed over 210 triples.

Parameters clean_unseen (*bool*) – If `True`, filters triples in validation and test sets that include entities not present in the training set.

Returns splits – The dataset splits: {'train': train, 'valid': valid, 'test': test}. Each split is an ndarray of shape [n, 3].

Return type dict

Examples

```
>>> from ampligraph.datasets import load_wn18rr
>>> X = load_wn18rr()
>>> X["valid"][0]
array(['02174461', '_hypernym', '02176268'], dtype=object)
```

Datasets Summary

Dataset	Train	Valid	Test	Entities	Relations
FB15K-237	272,115	17,535	20,466	14,541	237
WN18RR	86,835	3,034	3,134	40,943	11
FB15K	483,142	50,000	59,071	14,951	1,345
WN18	141,442	5,000	5,000	40,943	18
YAGO3-10	1,079,040	5,000	5,000	123,182	37

Hint: WN18 and FB15k include a large number of inverse relations, and its use in experiments has been deprecated. **Use WN18RR and FB15K-237 instead**.

Warning: FB15K-237's validation set contains 8 unseen entities over 9 triples. The test set has 29 unseen entities, distributed over 28 triples. WN18RR's validation set contains 198 unseen entities over 210 triples. The test set has 209 unseen entities, distributed over 210 triples.

Generic Loaders

Functions to load custom knowledge graphs from disk.

`load_from_csv`(directory_path, file_name[, ...])	Load a knowledge graph from a csv file
`load_from_ntriples`(folder_name, file_name[, ...])	Load RDF ntriples
`load_from_rdf`(folder_name, file_name[, ...])	Load an RDF file

load_from_csv

`ampligraph.datasets.load_from_csv`(*directory_path, file_name, sep='\t', header=None*)

Load a knowledge graph from a csv file

Loads a knowledge graph serialized in a csv file as:

```
subj1    relationX   obj1
subj1    relationY   obj2
subj3    relationZ   obj2
subj4    relationY   obj2
...
```

Note: The function filters duplicated statements.

Note: It is recommended to use *ampligraph.evaluation.train_test_split_no_unseen()* to split custom knowledge graphs into train, validation, and test sets. Using this function will lead to validation, test sets that do not include triples with entities that do not occur in the training set.

Parameters

- **directory_path** (*str*) – folder where the input file is stored.
- **file_name** (*str*) – file name
- **sep** (*str*) – The subject-predicate-object separator (default).
- **header** (*int, None*) – The row of the header of the csv file. Same as pandas.read_csv header param.

Returns **triples** – the actual triples of the file.

Return type ndarray , shape [n, 3]

Examples

```
>>> from ampligraph.datasets import load_from_csv
>>> X = load_from_csv('folder', 'dataset.csv', sep=',')
>>> X[:3]
array([['a', 'y', 'b'],
       ['b', 'y', 'a'],
       ['a', 'y', 'c']],
      dtype='<U1')
```

load_from_ntriples

ampligraph.datasets.**load_from_ntriples**(*folder_name*, *file_name*, *data_home=None*)

Load RDF ntriples

Loads an RDF knowledge graph serialized as ntriples, without building an RDF graph in memory. This function should be preferred over `load_from_rdf()`, since it does not load the graph into an rdflib model (and it is therefore faster by order of magnitudes). Nevertheless, it requires a ntriples serialization as in the example below:

```
_:alice <http://xmlns.com/foaf/0.1/knows> _:bob .
_:bob <http://xmlns.com/foaf/0.1/knows> _:alice .
```

Note: It is recommended to use *ampligraph.evaluation.train_test_split_no_unseen()* to split custom knowledge graphs into train, validation, and test sets. Using this function will lead to validation, test sets that do not include triples with entities that do not occur in the training set.

Parameters

- **folder_name** (*str*) – base folder where the file is stored.
- **file_name** (*str*) – file name

Returns **triples** – the actual triples of the file.

Return type ndarray , shape [n, 3]

load_from_rdf

`ampligraph.datasets.load_from_rdf(folder_name, file_name, format='nt', data_home=None)`

Load an RDF file

Loads an RDF knowledge graph using rdflib APIs. Multiple RDF serialization formats are supported (nt, ttl, rdf/xml, etc). The entire graph will be loaded in memory, and converted into an rdflib *Graph* object.

Warning: Large RDF graphs should be serialized to ntriples beforehand and loaded with `load_from_ntriples()` instead.

Note: It is recommended to use `ampligraph.evaluation.train_test_split_no_unseen()` to split custom knowledge graphs into train, validation, and test sets. Using this function will lead to validation, test sets that do not include triples with entities that do not occur in the training set.

Parameters

- **folder_name** (*str*) – base folder where the file is stored.
- **file_name** (*str*) – file name
- **format** (*str*) – The RDF serialization format (nt, ttl, rdf/xml - see rdflib documentation)

Returns **triples** – the actual triples of the file.

Return type ndarray , shape [n, 3]

Hint: AmpliGraph includes a helper function to split a generic knowledge graphs into **training**, **validation**, and **test** sets. See `ampligraph.evaluation.train_test_split_no_unseen()`.

3.3.2 Models

This module includes neural graph embedding models and support functions.

Knowledge graph embedding models are neural architectures that encode concepts from a knowledge graph (i.e. entities $\mathcal{E}$ and relation types $\mathcal{R}$) into low-dimensional, continuous vectors $\in \mathcal{R}^k$. Such *knowledge graph embeddings* have applications in knowledge graph completion, entity resolution, and link-based clustering, just to cite a few [NMTG16].

Knowledge Graph Embedding Models

`RandomBaseline`([seed])	Random baseline
`TransE`([k, eta, epochs, batches_count, . . .])	Translating Embeddings (TransE)
`DistMult`([k, eta, epochs, batches_count, . . .])	The DistMult model
`ComplEx`([k, eta, epochs, batches_count, . . .])	Complex embeddings (ComplEx)
`HolE`([k, eta, epochs, batches_count, seed, . . .])	Holographic Embeddings

RandomBaseline

class ampligraph.latent_features.**RandomBaseline**(*seed=0*)

Random baseline

A dummy model that assigns a pseudo-random score included between 0 and 1, drawn from a uniform distribution.

The model is useful whenever you need to compare the performance of another model on a custom knowledge graph, and no other baseline is available.

Note: Although the model still requires invoking the `fit()` method, no actual training will be carried out.

Examples

```
>>> import numpy as np
>>> from ampligraph.latent_features import RandomBaseline
>>> model = RandomBaseline()
>>> X = np.array([['a', 'y', 'b'],
>>>               ['b', 'y', 'a'],
>>>               ['a', 'y', 'c'],
>>>               ['c', 'y', 'a'],
>>>               ['a', 'y', 'd'],
>>>               ['c', 'y', 'd'],
>>>               ['b', 'y', 'c'],
>>>               ['f', 'y', 'e']])
>>> model.fit(X)
>>> model.predict(np.array([['f', 'y', 'e'], ['b', 'y', 'd']]))
[0.5488135039273248, 0.7151893663724195]
```

Methods

`__init__`([seed])	Initialize the model
`fit`(X)	Train the random model
`predict`(X[, from_idx, get_ranks])	Assign random scores to candidate triples and then ranks them

__init__(*seed=0*)

Initialize the model

Parameters **seed** (*int*) – The seed used by the internal random numbers generator.

fit(*X*)

Train the random model

Parameters **X** (*ndarray, shape [n, 3]*) – The training triples

predict(*X, from_idx=False, get_ranks=False*)

Assign random scores to candidate triples and then ranks them

Parameters

- **X** (*ndarray, shape [n, 3]*) – The triples to score.

- **from_idx** (*bool*) – If True, will skip conversion to internal IDs. (default: False).
- **get_ranks** (*bool*) – Flag to compute ranks by scoring against corruptions (default: False).

Returns

- **scores** (*ndarray, shape [n]*) – The predicted scores for input triples X.
- **ranks** (*ndarray, shape [n]*) – Rank of the triple

TransE

class ampligraph.latent_features.**TransE**(*k=100, eta=2, epochs=100, batches_count=100, seed=0, embedding_model_params={'corrupt_sides': ['s+o'], 'negative_corruption_entities': 'all', 'norm': 1, 'normalize_ent_emb': False}, optimizer='adam', optimizer_params={'lr': 0.0005}, loss='nll', loss_params={}, regularizer=None, regularizer_params={}, verbose=False*)

Translating Embeddings (TransE)

The model as described in [BUGD+13].

The scoring function of TransE computes a similarity between the embedding of the subject $\mathbf{e}_{sub}$ translated by the embedding of the predicate $\mathbf{e}_{pred}$ and the embedding of the object $\mathbf{e}_{obj}$, using the L_1 or L_2 norm $||\cdot||$:

$$f_{TransE} = -||\mathbf{e}_{sub} + \mathbf{e}_{pred} - \mathbf{e}_{obj}||_n$$

Such scoring function is then used on positive and negative triples t^+, t^- in the loss function.

Examples

```
>>> import numpy as np
>>> from ampligraph.latent_features import TransE
>>> model = TransE(batches_count=1, seed=555, epochs=20, k=10, loss='pairwise',
>>>                loss_params={'margin':5})
>>> X = np.array([['a', 'y', 'b'],
>>>               ['b', 'y', 'a'],
>>>               ['a', 'y', 'c'],
>>>               ['c', 'y', 'a'],
>>>               ['a', 'y', 'd'],
>>>               ['c', 'y', 'd'],
>>>               ['b', 'y', 'c'],
>>>               ['f', 'y', 'e']])
>>> model.fit(X)
>>> model.predict(np.array([['f', 'y', 'e'], ['b', 'y', 'd']]))
[-4.6903257, -3.9047198]
>>> model.get_embeddings(['f','e'], embedding_type='entity')
array([[ 0.10673896, -0.28916815,  0.6278883 , -0.1194713 , -0.10372276,
-0.37258488,  0.06460134, -0.27879423,  0.25456288,  0.18665907],
[-0.64494324, -0.12939683,  0.3181001 ,  0.16745451, -0.03766293,
 0.24314676, -0.23038973, -0.658638  ,  0.5680542 , -0.05401703]],
dtype=float32)
```

Methods

`__init__`([k, eta, epochs, batches_count, . . .])	Initialize an EmbeddingModel
`fit`(X[, early_stopping, early_stopping_params])	Train an Translating Embeddings model.
`get_embeddings`(entities[, embedding_type])	Get the embeddings of entities or relations.
`predict`(X[, from_idx, get_ranks])	Predict the scores of triples using a trained embedding model.

__init__(*k=100, eta=2, epochs=100, batches_count=100, seed=0, embedding_model_params={'corrupt_sides': ['s+o'], 'negative_corruption_entities': 'all', 'norm': 1, 'normalize_ent_emb': False}, optimizer='adam', optimizer_params={'lr': 0.0005}, loss='nll', loss_params={}, regularizer=None, regularizer_params={}, verbose=False*)

Initialize an EmbeddingModel

Also creates a new Tensorflow session for training.

Parameters

- **k** (*int*) – Embedding space dimensionality
- **eta** (*int*) – The number of negatives that must be generated at runtime during training for each positive.
- **epochs** (*int*) – The iterations of the training loop.
- **batches_count** (*int*) – The number of batches in which the training set must be split during the training loop.
- **seed** (*int*) – The seed used by the internal random numbers generator.
- **embedding_model_params** (*dict*) – TransE-specific hyperparams, passed to the model as a dictionary.

  Supported keys:

  – **'norm'** (int): the norm to be used in the scoring function (1 or 2-norm - default: 1).

  – **'normalize_ent_emb'** (bool): flag to indicate whether to normalize entity embeddings after each batch update (default: False).

  – **negative_corruption_entities** : entities to be used for generation of corruptions while training. It can take the following values : `all` (default: all entities), `batch` (entities present in each batch), list of entities or an int (which indicates how many entities that should be used for corruption generation).

  – **corrupt_sides** : Specifies how to generate corruptions for training. Takes values *s*, *o*, *s+o* or any combination passed as a list

  Example: `embedding_model_params={'norm': 1, 'normalize_ent_emb': False}`

- **optimizer** (*string*) – The optimizer used to minimize the loss function. Choose between 'sgd', 'adagrad', 'adam', 'momentum'.
- **optimizer_params** (*dict*) – Arguments specific to the optimizer, passed as a dictionary.

  Supported keys:

  – **'lr'** (float): learning rate (used by all the optimizers). Default: 0.1.

  - **'momentum'** (float): learning momentum (only used when `optimizer=momentum`). Default: 0.9.

  Example: `optimizer_params={'lr': 0.01}`

- **loss** (*string*) – The type of loss function to use during training.
  - `pairwise` the model will use pairwise margin-based loss function.
  - `nll` the model will use negative loss likelihood.
  - `absolute_margin` the model will use absolute margin likelihood.
  - `self_adversarial` the model will use adversarial sampling loss function.
  - `multiclass_nll` the model will use multiclass nll loss. Switch to multiclass loss defined in [aC15] by passing 'corrupt_sides' as ['s','o'] to embedding_model_params. To use loss defined in [KBK17] pass 'corrupt_sides' as 'o' to embedding_model_params
- **loss_params** (*dict*) – Dictionary of loss-specific hyperparameters. See *loss functions* documentation for additional details.

  Example: `optimizer_params={'lr': 0.01}` if `loss='pairwise'`.
- **regularizer** (*string*) – The regularization strategy to use with the loss function.
  - `None`: the model will not use any regularizer (default)
  - 'LP': the model will use L1, L2 or L3 based on the value of `regularizer_params['p']` (see below).
- **regularizer_params** (*dict*) – Dictionary of regularizer-specific hyperparameters. See the *regularizers* documentation for additional details.

  Example: `regularizer_params={'lambda': 1e-5, 'p': 2}` if `regularizer='LP'`.
- **verbose** (*bool*) – Verbose mode

fit (*X*, *early_stopping=False*, *early_stopping_params={}*)
Train an Translating Embeddings model.

The model is trained on a training set X using the training protocol described in [TWR+16].

Parameters

- **X** (*ndarray, shape [n, 3]*) – The training triples
- **early_stopping** (*bool*) – Flag to enable early stopping (default:False).

  If set to `True`, the training loop adopts the following early stopping heuristic:
  - The model will be trained regardless of early stopping for `burn_in` epochs.
  - Every `check_interval` epochs the method will compute the metric specified in `criteria`.

  If such metric decreases for `stop_interval` checks, we stop training early.

  Note the metric is computed on `x_valid`. This is usually a validation set that you held out.

  Also, because `criteria` is a ranking metric, it requires generating negatives. Entities used to generate corruptions can be specified, as long as the side(s) of a triple to corrupt. The method supports filtered metrics, by passing an array of positives to `x_filter`. This will be used to filter the negatives generated on the fly (i.e. the corruptions).

Note: Keep in mind the early stopping criteria may introduce a certain overhead (caused by the metric computation). The goal is to strike a good trade-off between such overhead and saving training epochs.

A common approach is to use MRR unfiltered:

```
early_stopping_params={x_valid=X['valid'], 'criteria': 'mrr'}
```

Note the size of validation set also contributes to such overhead. In most cases a smaller validation set would be enough.

- **early_stopping_params** (*dictionary*) – Dictionary of hyperparameters for the early stopping heuristics.

  The following string keys are supported:

  - **'x_valid'**: ndarray, shape [n, 3] : Validation set to be used for early stopping.
  - **'criteria'**: string : criteria for early stopping 'hits10', 'hits3', 'hits1' or 'mrr'(default).
  - **'x_filter'**: ndarray, shape [n, 3] : Positive triples to use as filter if a 'filtered' early stopping criteria is desired (i.e. filtered-MRR if 'criteria':'mrr'). Note this will affect training time (no filter by default).
  - **'burn_in'**: int : Number of epochs to pass before kicking in early stopping (default: 100).
  - **check_interval'**: int : Early stopping interval after burn-in (default:10).
  - **'stop_interval'**: int : Stop if criteria is performing worse over n consecutive checks (default: 3)
  - **'corruption_entities'**: List of entities to be used for corruptions. If 'all', it uses all entities (default: 'all')
  - **'corrupt_side'**: Specifies which side to corrupt. 's', 'o', 's+o' (default)

  Example: `early_stopping_params={x_valid=X['valid'], 'criteria': 'mrr'}`

get_embeddings (*entities*, *embedding_type='entity'*)
Get the embeddings of entities or relations.

Parameters

- **entities** (*array-like, dtype=int, shape=[n]*) – The entities (or relations) of interest. Element of the vector must be the original string literals, and not internal IDs.
- **embedding_type** (*string*) – If 'entity', the `entities` argument will be considered as a list of knowledge graph entities (i.e. nodes). If set to 'relation', they will be treated as relation types instead (i.e. predicates).

Returns **embeddings** – An array of k-dimensional embeddings.

Return type ndarray, shape [n, k]

predict (*X*, *from_idx=False*, *get_ranks=False*)
Predict the scores of triples using a trained embedding model.

The function returns raw scores generated by the model.

Note: To obtain probability estimates, use a logistic sigmoid:

```
>>> model.fit(X)
>>> y_pred = model.predict(np.array([['f', 'y', 'e'], ['b', 'y', 'd
↪']]))
>>> print(y_pred)
[-4.6903257, -3.9047198]
>>> from scipy.special import expit
>>> expit(y_pred)
array([0.00910012, 0.01974873], dtype=float32)
```

Parameters

- **X** (*ndarray, shape [n, 3]*) – The triples to score.
- **from_idx** (*bool*) – If True, will skip conversion to internal IDs. (default: False).
- **get_ranks** (*bool*) – Flag to compute ranks by scoring against corruptions (default: False).

Returns

- **scores_predict** (*ndarray, shape [n]*) – The predicted scores for input triples X.
- **rank** (*ndarray, shape [n]*) – Ranks of the triples (only returned if `get_ranks=True`.

DistMult

class ampligraph.latent_features.**DistMult**(*k=100, eta=2, epochs=100, batches_count=100, seed=0, embedding_model_params={'corrupt_sides': ['s+o'], 'negative_corruption_entities': 'all', 'normalize_ent_emb': False}, optimizer='adam', optimizer_params={'lr': 0.0005}, loss='nll', loss_params={}, regularizer=None, regularizer_params={}, verbose=False*)

The DistMult model

The model as described in [YYH+14].

The bilinear diagonal DistMult model uses the trilinear dot product as scoring function:

$$f_{DistMult} = \langle \mathbf{r}_p, \mathbf{e}_s, \mathbf{e}_o \rangle$$

where $\mathbf{e}_s$ is the embedding of the subject, $\mathbf{r}_p$ the embedding of the predicate and $\mathbf{e}_o$ the embedding of the object.

Examples

```
>>> import numpy as np
>>> from ampligraph.latent_features import DistMult
>>> model = DistMult(batches_count=1, seed=555, epochs=20, k=10, loss='pairwise',
```

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```
>>>          loss_params={'margin':5})
>>> X = np.array([['a', 'y', 'b'],
>>>               ['b', 'y', 'a'],
>>>               ['a', 'y', 'c'],
>>>               ['c', 'y', 'a'],
>>>               ['a', 'y', 'd'],
>>>               ['c', 'y', 'd'],
>>>               ['b', 'y', 'c'],
>>>               ['f', 'y', 'e']])
>>> model.fit(X)
>>> model.predict(np.array([['f', 'y', 'e'], ['b', 'y', 'd']]))
[-0.13863425, -0.09917116]
>>> model.get_embeddings(['f','e'], embedding_type='entity')
array([[ 0.10137264, -0.28248304,  0.6153027 , -0.13133956, -0.11675504,
-0.37876177,  0.06027773, -0.26390398,  0.254603  ,  0.1888549 ],
[-0.6467299 , -0.13729756,  0.3074872 ,  0.16966867, -0.04098966,
 0.25289047, -0.2212451 , -0.6527815 ,  0.5657673 , -0.03876532]],
dtype=float32)
```

Methods

__init__([k, eta, epochs, batches_count, . . .])	Initialize an EmbeddingModel
fit(X[, early_stopping, early_stopping_params])	Train an DistMult.
get_embeddings(entities[, embedding_type])	Get the embeddings of entities or relations.
predict(X[, from_idx, get_ranks])	Predict the scores of triples using a trained embedding model.

__init__(*k=100, eta=2, epochs=100, batches_count=100, seed=0, embedding_model_params={'corrupt_sides': ['s+o'], 'negative_corruption_entities': 'all', 'normalize_ent_emb': False}, optimizer='adam', optimizer_params={'lr': 0.0005}, loss='nll', loss_params={}, regularizer=None, regularizer_params={}, verbose=False*)
Initialize an EmbeddingModel

Also creates a new Tensorflow session for training.

Parameters

- **k** (*int*) – Embedding space dimensionality
- **eta** (*int*) – The number of negatives that must be generated at runtime during training for each positive.
- **epochs** (*int*) – The iterations of the training loop.
- **batches_count** (*int*) – The number of batches in which the training set must be split during the training loop.
- **seed** (*int*) – The seed used by the internal random numbers generator.
- **embedding_model_params** (*dict*) – DistMult-specific hyperparams, passed to the model as a dictionary.

  Supported keys:

  – **'normalize_ent_emb'** (bool): flag to indicate whether to normalize entity embeddings after each batch update (default: False).

- **'negative_corruption_entities'** - Entities to be used for generation of corruptions while training. It can take the following values : `all` (default: all entities), `batch` (entities present in each batch), list of entities or an int (which indicates how many entities that should be used for corruption generation).
- **corrupt_sides** : Specifies how to generate corruptions for training. Takes values *s*, *o*, *s+o* or any combination passed as a list

Example: `embedding_model_params={'normalize_ent_emb': False}`

- **optimizer** (*string*) – The optimizer used to minimize the loss function. Choose between 'sgd', 'adagrad', 'adam', 'momentum'.
- **optimizer_params** (*dict*) – Arguments specific to the optimizer, passed as a dictionary.

  Supported keys:

  - **'lr'** (float): learning rate (used by all the optimizers). Default: 0.1.
  - **'momentum'** (float): learning momentum (only used when `optimizer=momentum`). Default: 0.9.

  Example: `optimizer_params={'lr': 0.01}`

- **loss** (*string*) – The type of loss function to use during training.
  - `pairwise` the model will use pairwise margin-based loss function.
  - `nll` the model will use negative loss likelihood.
  - `absolute_margin` the model will use absolute margin likelihood.
  - `self_adversarial` the model will use adversarial sampling loss function.
  - `multiclass_nll` the model will use multiclass nll loss. Switch to multiclass loss defined in [aC15] by passing 'corrupt_sides' as ['s','o'] to embedding_model_params. To use loss defined in [KBK17] pass 'corrupt_sides' as 'o' to embedding_model_params
- **loss_params** (*dict*) – Dictionary of loss-specific hyperparameters. See *loss functions* documentation for additional details.

  Example: `optimizer_params={'lr': 0.01}` if `loss='pairwise'`.

- **regularizer** (*string*) – The regularization strategy to use with the loss function.
  - `None`: the model will not use any regularizer (default)
  - 'LP': the model will use L1, L2 or L3 based on the value of `regularizer_params['p']` (see below).
- **regularizer_params** (*dict*) – Dictionary of regularizer-specific hyperparameters. See the *regularizers* documentation for additional details.

  Example: `regularizer_params={'lambda': 1e-5, 'p': 2}` if `regularizer='LP'`.

- **verbose** (*bool*) – Verbose mode

fit (*X*, *early_stopping=False*, *early_stopping_params={}*)
Train an DistMult.

The model is trained on a training set X using the training protocol described in [TWR+16].

Parameters

- **X** (*ndarray, shape [n, 3]*) – The training triples
- **early_stopping** (*bool*) – Flag to enable early stopping (default:False).

  If set to `True`, the training loop adopts the following early stopping heuristic:

  – The model will be trained regardless of early stopping for `burn_in` epochs.

  – Every `check_interval` epochs the method will compute the metric specified in `criteria`.

  If such metric decreases for `stop_interval` checks, we stop training early.

  Note the metric is computed on `x_valid`. This is usually a validation set that you held out.

  Also, because `criteria` is a ranking metric, it requires generating negatives. Entities used to generate corruptions can be specified, as long as the side(s) of a triple to corrupt. The method supports filtered metrics, by passing an array of positives to `x_filter`. This will be used to filter the negatives generated on the fly (i.e. the corruptions).

  Note: Keep in mind the early stopping criteria may introduce a certain overhead (caused by the metric computation). The goal is to strike a good trade-off between such overhead and saving training epochs.

  A common approach is to use MRR unfiltered:

  ```
  early_stopping_params={x_valid=X['valid'], 'criteria': 'mrr'}
  ```

  Note the size of validation set also contributes to such overhead. In most cases a smaller validation set would be enough.

- **early_stopping_params** (*dictionary*) – Dictionary of hyperparameters for the early stopping heuristics.

  The following string keys are supported:

  – **'x_valid'**: ndarray, shape [n, 3] : Validation set to be used for early stopping.

  – **'criteria'**: string : criteria for early stopping 'hits10', 'hits3', 'hits1' or 'mrr'(default).

  – **'x_filter'**: ndarray, shape [n, 3] : Positive triples to use as filter if a 'filtered' early stopping criteria is desired (i.e. filtered-MRR if 'criteria':'mrr'). Note this will affect training time (no filter by default).

  – **'burn_in'**: int : Number of epochs to pass before kicking in early stopping (default: 100).

  – **check_interval'**: int : Early stopping interval after burn-in (default:10).

  – **'stop_interval'**: int : Stop if criteria is performing worse over n consecutive checks (default: 3)

  – **'corruption_entities'**: List of entities to be used for corruptions. If 'all', it uses all entities (default: 'all')

– **'corrupt_side'**: Specifies which side to corrupt. 's', 'o', 's+o' (default)

Example: `early_stopping_params={x_valid=X['valid'], 'criteria': 'mrr'}`

get_embeddings (*entities*, *embedding_type='entity'*)

Get the embeddings of entities or relations.

Parameters

- **entities** (*array-like, dtype=int, shape=[n]*) – The entities (or relations) of interest. Element of the vector must be the original string literals, and not internal IDs.
- **embedding_type** (*string*) – If 'entity', the `entities` argument will be considered as a list of knowledge graph entities (i.e. nodes). If set to 'relation', they will be treated as relation types instead (i.e. predicates).

Returns **embeddings** – An array of k-dimensional embeddings.

Return type ndarray, shape [n, k]

predict (*X*, *from_idx=False*, *get_ranks=False*)

Predict the scores of triples using a trained embedding model.

The function returns raw scores generated by the model.

Note: To obtain probability estimates, use a logistic sigmoid:

```
>>> model.fit(X)
>>> y_pred = model.predict(np.array([['f', 'y', 'e'], ['b', 'y', 'd
↪']]))
>>> print(y_pred)
[-0.13863425, -0.09917116]
>>> from scipy.special import expit
>>> expit(y_pred)
array([0.4653968 , 0.47522753], dtype=float32)
```

Parameters

- **X** (*ndarray, shape [n, 3]*) – The triples to score.
- **from_idx** (*bool*) – If True, will skip conversion to internal IDs. (default: False).
- **get_ranks** (*bool*) – Flag to compute ranks by scoring against corruptions (default: False).

Returns

- **scores_predict** (*ndarray, shape [n]*) – The predicted scores for input triples X.
- **rank** (*ndarray, shape [n]*) – Ranks of the triples (only returned if `get_ranks=True`.

ComplEx

class ampligraph.latent_features.**ComplEx**(*k=100, eta=2, epochs=100, batches_count=100, seed=0, embedding_model_params={'corrupt_sides': ['s+o'], 'negative_corruption_entities': 'all'}, optimizer='adam', optimizer_params={'lr': 0.0005}, loss='nll', loss_params={}, regularizer=None, regularizer_params={}, verbose=False*)

Complex embeddings (ComplEx)

The ComplEx model [TWR+16] is an extension of the `ampligraph.latent_features.DistMult` bilinear diagonal model . ComplEx scoring function is based on the trilinear Hermitian dot product in $\mathcal{C}$:

$$f_{ComplEx} = Re(\langle \mathbf{r}_p, \mathbf{e}_s, \overline{\mathbf{e}_o} \rangle)$$

Note that because embeddings are in $\mathcal{C}$, ComplEx uses twice as many parameters as `ampligraph.latent_features.DistMult`.

Examples

```
>>> import numpy as np
>>> from ampligraph.latent_features import ComplEx
>>>
>>> model = ComplEx(batches_count=1, seed=555, epochs=20, k=10,
>>>             loss='pairwise', loss_params={'margin':1},
>>>             regularizer='LP', regularizer_params={'lambda':0.1})
>>> X = np.array([['a', 'y', 'b'],
>>>               ['b', 'y', 'a'],
>>>               ['a', 'y', 'c'],
>>>               ['c', 'y', 'a'],
>>>               ['a', 'y', 'd'],
>>>               ['c', 'y', 'd'],
>>>               ['b', 'y', 'c'],
>>>               ['f', 'y', 'e']])
>>> model.fit(X)
>>> model.predict(np.array([['f', 'y', 'e'], ['b', 'y', 'd']]))
[-0.31336197, 0.07829369]
>>> model.get_embeddings(['f','e'], embedding_type='entity')
array([[ 0.17496692,  0.15856805,  0.2549046 ,  0.21418071, -0.00980021,
0.06208976, -0.2573946 ,  0.01115128, -0.10728686,  0.40512595,
-0.12340491, -0.11021495,  0.28515074,  0.34275156,  0.58547366,
0.03383447, -0.37839213,  0.1353071 ,  0.50376487, -0.26477185],
[-0.19194135,  0.20568603,  0.04714957,  0.4366147 ,  0.07175589,
 0.5740745 ,  0.28201544,  0.3266275 , -0.06701915,  0.29062983,
-0.21265475,  0.5720126 , -0.05321272,  0.04141249,  0.01574909,
-0.11786222,  0.30488515,  0.34970865,  0.23362857, -0.55025095]],
dtype=float32)
```

Methods

`__init__`([k, eta, epochs, batches_count, ...])	Initialize an EmbeddingModel
`fit`(X[, early_stopping, early_stopping_params])	Train a ComplEx model.
`get_embeddings`(entities[, embedding_type])	Get the embeddings of entities or relations.
`predict`(X[, from_idx, get_ranks])	Predict the scores of triples using a trained embedding model.

__init__(*k=100, eta=2, epochs=100, batches_count=100, seed=0, embedding_model_params={'corrupt_sides': ['s+o'], 'negative_corruption_entities': 'all'}, optimizer='adam', optimizer_params={'lr': 0.0005}, loss='nll', loss_params={}, regularizer=None, regularizer_params={}, verbose=False*)

Initialize an EmbeddingModel

Also creates a new Tensorflow session for training.

Parameters

- **k** (*int*) – Embedding space dimensionality
- **eta** (*int*) – The number of negatives that must be generated at runtime during training for each positive.
- **epochs** (*int*) – The iterations of the training loop.
- **batches_count** (*int*) – The number of batches in which the training set must be split during the training loop.
- **seed** (*int*) – The seed used by the internal random numbers generator.
- **embedding_model_params** (*dict*) – ComplEx-specific hyperparams:
  - **'negative_corruption_entities'** - Entities to be used for generation of corruptions while training. It can take the following values : `all` (default: all entities), `batch` (entities present in each batch), list of entities or an int (which indicates how many entities that should be used for corruption generation).
  - **corrupt_sides** : Specifies how to generate corruptions for training. Takes values *s*, *o*, *s+o* or any combination passed as a list
- **optimizer** (*string*) – The optimizer used to minimize the loss function. Choose between 'sgd', 'adagrad', 'adam', 'momentum'.
- **optimizer_params** (*dict*) – Arguments specific to the optimizer, passed as a dictionary.

  Supported keys:

  - **'lr'** (float): learning rate (used by all the optimizers). Default: 0.1.
  - **'momentum'** (float): learning momentum (only used when `optimizer=momentum`). Default: 0.9.

  Example: `optimizer_params={'lr': 0.01}`
- **loss** (*string*) – The type of loss function to use during training.
  - `pairwise` the model will use pairwise margin-based loss function.
  - `nll` the model will use negative loss likelihood.
  - `absolute_margin` the model will use absolute margin likelihood.
  - `self_adversarial` the model will use adversarial sampling loss function.

 - `multiclass_nll` the model will use multiclass nll loss. Switch to multiclass loss defined in [aC15] by passing 'corrupt_sides' as ['s','o'] to embedding_model_params. To use loss defined in [KBK17] pass 'corrupt_sides' as 'o' to embedding_model_params

- **loss_params** (*dict*) – Dictionary of loss-specific hyperparameters. See *loss functions* documentation for additional details.

  Example: `optimizer_params={'lr': 0.01}` if `loss='pairwise'`.

- **regularizer** (*string*) – The regularization strategy to use with the loss function.

  - `None`: the model will not use any regularizer (default)
  - 'LP': the model will use L1, L2 or L3 based on the value of `regularizer_params['p']` (see below).

- **regularizer_params** (*dict*) – Dictionary of regularizer-specific hyperparameters. See the *regularizers* documentation for additional details.

  Example: `regularizer_params={'lambda': 1e-5, 'p': 2}` if `regularizer='LP'`.

- **verbose** (*bool*) – Verbose mode

fit(*X*, *early_stopping=False*, *early_stopping_params={}*)

Train a ComplEx model.

The model is trained on a training set X using the training protocol described in [TWR+16].

Parameters

- **X** (*ndarray, shape [n, 3]*) – The training triples
- **early_stopping** (*bool*) – Flag to enable early stopping (default:False).

  If set to `True`, the training loop adopts the following early stopping heuristic:

  - The model will be trained regardless of early stopping for `burn_in` epochs.
  - Every `check_interval` epochs the method will compute the metric specified in `criteria`.

  If such metric decreases for `stop_interval` checks, we stop training early.

  Note the metric is computed on `x_valid`. This is usually a validation set that you held out.

  Also, because `criteria` is a ranking metric, it requires generating negatives. Entities used to generate corruptions can be specified, as long as the side(s) of a triple to corrupt. The method supports filtered metrics, by passing an array of positives to `x_filter`. This will be used to filter the negatives generated on the fly (i.e. the corruptions).

  Note: Keep in mind the early stopping criteria may introduce a certain overhead (caused by the metric computation). The goal is to strike a good trade-off between such overhead and saving training epochs.

  A common approach is to use MRR unfiltered:

```
early_stopping_params={x_valid=X['valid'], 'criteria': 'mrr'}
```

Note the size of validation set also contributes to such overhead. In most cases a smaller validation set would be enough.

- **early_stopping_params** (*dictionary*) – Dictionary of hyperparameters for the early stopping heuristics.

  The following string keys are supported:

  - **'x_valid'**: ndarray, shape [n, 3] : Validation set to be used for early stopping.
  - **'criteria'**: string : criteria for early stopping 'hits10', 'hits3', 'hits1' or 'mrr'(default).
  - **'x_filter'**: ndarray, shape [n, 3] : Positive triples to use as filter if a 'filtered' early stopping criteria is desired (i.e. filtered-MRR if 'criteria':'mrr'). Note this will affect training time (no filter by default).
  - **'burn_in'**: int : Number of epochs to pass before kicking in early stopping (default: 100).
  - **check_interval'**: int : Early stopping interval after burn-in (default:10).
  - **'stop_interval'**: int : Stop if criteria is performing worse over n consecutive checks (default: 3)
  - **'corruption_entities'**: List of entities to be used for corruptions. If 'all', it uses all entities (default: 'all')
  - **'corrupt_side'**: Specifies which side to corrupt. 's', 'o', 's+o' (default)

  Example: `early_stopping_params={x_valid=X['valid'], 'criteria': 'mrr'}`

get_embeddings (*entities*, *embedding_type='entity'*)
Get the embeddings of entities or relations.

Parameters

- **entities** (*array-like, dtype=int, shape=[n]*) – The entities (or relations) of interest. Element of the vector must be the original string literals, and not internal IDs.
- **embedding_type** (*string*) – If 'entity', the `entities` argument will be considered as a list of knowledge graph entities (i.e. nodes). If set to 'relation', they will be treated as relation types instead (i.e. predicates).

Returns **embeddings** – An array of k-dimensional embeddings.

Return type ndarray, shape [n, k]

predict (*X*, *from_idx=False*, *get_ranks=False*)
Predict the scores of triples using a trained embedding model.

The function returns raw scores generated by the model.

Note: To obtain probability estimates, use a logistic sigmoid:

```
>>> model.fit(X)
>>> y_pred = model.predict(np.array([['f', 'y', 'e'], ['b', 'y', 'd
↪']]))
>>> print(y_pred)
[-0.31336197, 0.07829369]
>>> from scipy.special import expit
>>> expit(y_pred)
array([0.42229432, 0.51956344], dtype=float32)
```

Parameters

- **X** (*ndarray, shape [n, 3]*) – The triples to score.
- **from_idx** (*bool*) – If True, will skip conversion to internal IDs. (default: False).
- **get_ranks** (*bool*) – Flag to compute ranks by scoring against corruptions (default: False).

Returns

- **scores_predict** (*ndarray, shape [n]*) – The predicted scores for input triples X.
- **rank** (*ndarray, shape [n]*) – Ranks of the triples (only returned if `get_ranks=True`.

HolE

class ampligraph.latent_features.**HolE**(*k=100, eta=2, epochs=100, batches_count=100, seed=0, embedding_model_params={'corrupt_sides': ['s+o'], 'negative_corruption_entities': 'all'}, optimizer='adam', optimizer_params={'lr': 0.0005}, loss='nll', loss_params={}, regularizer=None, regularizer_params={}, verbose=False*)

Holographic Embeddings

The HolE model [NRP+16] as re-defined by Hayashi et al. [HS17]:

$$f_{HolE} = \frac{2}{n} f_{ComplEx}$$

Examples

```
>>> import numpy as np
>>> from ampligraph.latent_features import HolE
>>> model = HolE(batches_count=1, seed=555, epochs=20, k=10,
>>>             loss='pairwise', loss_params={'margin':1},
>>>             regularizer='LP', regularizer_params={'lambda':0.1})
>>>
>>> X = np.array([['a', 'y', 'b'],
>>>               ['b', 'y', 'a'],
>>>               ['a', 'y', 'c'],
>>>               ['c', 'y', 'a'],
>>>               ['a', 'y', 'd'],
>>>               ['c', 'y', 'd'],
```

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```
>>>                ['b', 'y', 'c'],
>>>                ['f', 'y', 'e']])
>>> model.fit(X)
>>> model.predict(np.array([['f', 'y', 'e'], ['b', 'y', 'd']]), get_ranks=True)
([-0.06213863, 0.01563319], [13, 3])
>>> model.get_embeddings(['f','e'], embedding_type='entity')
    array([[ 0.17335348,  0.15826802,  0.24862595,  0.21404941, -0.00968813,
     0.06185953, -0.24956754,  0.01114257, -0.1038138 ,  0.40461722,
    -0.12298391, -0.10997348,  0.28220937,  0.34238952,  0.58363295,
     0.03315138, -0.37830347,  0.13480346,  0.49922466, -0.26328272],
    [-0.19098252,  0.20133668,  0.04635337,  0.4364128 ,  0.07014864,
     0.5713923 ,  0.28131518,  0.31721675, -0.06636801,  0.2848032 ,
    -0.2121708 ,  0.56917167, -0.05311433,  0.03093261,  0.01571475,
    -0.11373658,  0.29417998,  0.34896123,  0.22993243, -0.5499186 ]],
    dtype=float32)
```

Methods

`__init__`([k, eta, epochs, batches_count, . . .])	Initialize an EmbeddingModel
`fit`(X[, early_stopping, early_stopping_params])	Train a HolE model.
`get_embeddings`(entities[, embedding_type])	Get the embeddings of entities or relations.
`predict`(X[, from_idx, get_ranks])	Predict the scores of triples using a trained embedding model.

`__init__`(*k=100, eta=2, epochs=100, batches_count=100, seed=0, embedding_model_params={'corrupt_sides': ['s+o'], 'negative_corruption_entities': 'all'}, optimizer='adam', optimizer_params={'lr': 0.0005}, loss='nll', loss_params={}, regularizer=None, regularizer_params={}, verbose=False*)

Initialize an EmbeddingModel

Also creates a new Tensorflow session for training.

Parameters

- **k** (*int*) – Embedding space dimensionality
- **eta** (*int*) – The number of negatives that must be generated at runtime during training for each positive.
- **epochs** (*int*) – The iterations of the training loop.
- **batches_count** (*int*) – The number of batches in which the training set must be split during the training loop.
- **seed** (*int*) – The seed used by the internal random numbers generator.
- **embedding_model_params** (*dict*) – HolE-specific hyperparams:
  - **negative_corruption_entities** - Entities to be used for generation of corruptions while training. It can take the following values : `all` (default: all entities), `batch` (entities present in each batch), list of entities or an int (which indicates how many entities that should be used for corruption generation).
  - **corrupt_sides** : Specifies how to generate corruptions for training. Takes values *s*, *o*, *s+o* or any combination passed as a list

- **optimizer** (*string*) – The optimizer used to minimize the loss function. Choose between 'sgd', 'adagrad', 'adam', 'momentum'.
- **optimizer_params** (*dict*) – Arguments specific to the optimizer, passed as a dictionary.

  Supported keys:

  - **'lr'** (float): learning rate (used by all the optimizers). Default: 0.1.
  - **'momentum'** (float): learning momentum (only used when `optimizer=momentum`). Default: 0.9.

  Example: `optimizer_params={'lr': 0.01}`
- **loss** (*string*) – The type of loss function to use during training.
  - `pairwise` the model will use pairwise margin-based loss function.
  - `nll` the model will use negative loss likelihood.
  - `absolute_margin` the model will use absolute margin likelihood.
  - `self_adversarial` the model will use adversarial sampling loss function.
  - `multiclass_nll` the model will use multiclass nll loss. Switch to multiclass loss defined in [aC15] by passing 'corrupt_sides' as ['s','o'] to embedding_model_params. To use loss defined in [KBK17] pass 'corrupt_sides' as 'o' to embedding_model_params
- **loss_params** (*dict*) – Dictionary of loss-specific hyperparameters. See *loss functions* documentation for additional details.

  Example: `optimizer_params={'lr': 0.01}` if `loss='pairwise'`.
- **regularizer** (*string*) – The regularization strategy to use with the loss function.
  - `None`: the model will not use any regularizer (default)
  - 'LP': the model will use L1, L2 or L3 based on the value of `regularizer_params['p']` (see below).
- **regularizer_params** (*dict*) – Dictionary of regularizer-specific hyperparameters. See the *regularizers* documentation for additional details.

  Example: `regularizer_params={'lambda': 1e-5, 'p': 2}` if `regularizer='LP'`.
- **verbose** (*bool*) – Verbose mode

fit (*X*, *early_stopping=False*, *early_stopping_params={}*)
Train a HolE model.

The model is trained on a training set X using the training protocol described in [NRP+16].

Parameters

- **X** (*ndarray, shape [n, 3]*) – The training triples
- **early_stopping** (*bool*) – Flag to enable early stopping (default:False).

  If set to `True`, the training loop adopts the following early stopping heuristic:

  - The model will be trained regardless of early stopping for `burn_in` epochs.

– Every `check_interval` epochs the method will compute the metric specified in `criteria`.

If such metric decreases for `stop_interval` checks, we stop training early.

Note the metric is computed on `x_valid`. This is usually a validation set that you held out.

Also, because `criteria` is a ranking metric, it requires generating negatives. Entities used to generate corruptions can be specified, as long as the side(s) of a triple to corrupt. The method supports filtered metrics, by passing an array of positives to `x_filter`. This will be used to filter the negatives generated on the fly (i.e. the corruptions).

Note: Keep in mind the early stopping criteria may introduce a certain overhead (caused by the metric computation). The goal is to strike a good trade-off between such overhead and saving training epochs.

A common approach is to use MRR unfiltered:

```
early_stopping_params={x_valid=X['valid'], 'criteria': 'mrr'}
```

Note the size of validation set also contributes to such overhead. In most cases a smaller validation set would be enough.

- **early_stopping_params** (*dictionary*) – Dictionary of hyperparameters for the early stopping heuristics.

  The following string keys are supported:

  – **'x_valid'**: ndarray, shape [n, 3] : Validation set to be used for early stopping.

  – **'criteria'**: string : criteria for early stopping 'hits10', 'hits3', 'hits1' or 'mrr'(default).

  – **'x_filter'**: ndarray, shape [n, 3] : Positive triples to use as filter if a 'filtered' early stopping criteria is desired (i.e. filtered-MRR if 'criteria':'mrr'). Note this will affect training time (no filter by default).

  – **'burn_in'**: int : Number of epochs to pass before kicking in early stopping (default: 100).

  – **check_interval'**: int : Early stopping interval after burn-in (default:10).

  – **'stop_interval'**: int : Stop if criteria is performing worse over n consecutive checks (default: 3)

  – **'corruption_entities'**: List of entities to be used for corruptions. If 'all', it uses all entities (default: 'all')

  – **'corrupt_side'**: Specifies which side to corrupt. 's', 'o', 's+o' (default)

  Example: `early_stopping_params={x_valid=X['valid'], 'criteria': 'mrr'}`

get_embeddings (*entities*, *embedding_type='entity'*)

Get the embeddings of entities or relations.

Parameters

- **entities** (*array-like, dtype=int, shape=[n]*) – The entities (or relations) of interest. Element of the vector must be the original string literals, and not internal IDs.
- **embedding_type** (*string*) – If 'entity', the `entities` argument will be considered as a list of knowledge graph entities (i.e. nodes). If set to 'relation', they will be treated as relation types instead (i.e. predicates).

Returns **embeddings** – An array of k-dimensional embeddings.

Return type ndarray, shape [n, k]

predict (*X*, *from_idx=False*, *get_ranks=False*)

Predict the scores of triples using a trained embedding model.

The function returns raw scores generated by the model.

Note: To obtain probability estimates, use a logistic sigmoid:

```
>>> model.fit(X)
>>> y_pred = model.predict(np.array([['f', 'y', 'e'], ['b', 'y', 'd
↪']]))
>>> print(y_pred)
[-0.06213863, 0.01563319]
>>> from scipy.special import expit
>>> expit(y_pred)
array([0.48447034, 0.5039082 ], dtype=float32)
```

Parameters

- **X** (*ndarray, shape [n, 3]*) – The triples to score.
- **from_idx** (*bool*) – If True, will skip conversion to internal IDs. (default: False).
- **get_ranks** (*bool*) – Flag to compute ranks by scoring against corruptions (default: False).

Returns

- **scores_predict** (*ndarray, shape [n]*) – The predicted scores for input triples X.
- **rank** (*ndarray, shape [n]*) – Ranks of the triples (only returned if `get_ranks=True`.

Anatomy of a Model

Knowledge graph embeddings are learned by training a neural architecture over a graph. Although such architectures vary, the training phase always consists in minimizing a *loss function* $\mathcal{L}$ that includes a *scoring function* $f_m(t)$, i.e. a model-specific function that assigns a score to a triple $t = (sub, pred, obj)$.

AmpliGraph models include the following components:

- *Scoring function* $f(t)$
- *Loss function* $\mathcal{L}$
- *Optimization algorithm*
- *Negatives generation strategy*

AmpliGraph comes with a number of such components. They can be used in any combination to come up with a model that performs sufficiently well for the dataset of choice.

AmpliGraph features a number of abstract classes that can be extended to design new models:

EmbeddingModel([k, eta, epochs, ...])	Abstract class for embedding models
Loss(eta, hyperparam_dict[, verbose])	Abstract class for loss function.
Regularizer(hyperparam_dict[, verbose])	Abstract class for Regularizer.

EmbeddingModel

class ampligraph.latent_features.**EmbeddingModel**(*k=100*, *eta=2*, *epochs=100*, *batches_count=100*, *seed=0*, *embedding_model_params={}*, *optimizer='adam'*, *optimizer_params={'lr': 0.0005}*, *loss='nll'*, *loss_params={}*, *regularizer=None*, *regularizer_params={}*, *verbose=False*)

Abstract class for embedding models

AmpliGraph neural knowledge graph embeddings models extend this class and its core methods.

Methods

__init__([k, eta, epochs, batches_count, ...])	Initialize an EmbeddingModel
fit(X[, early_stopping, early_stopping_params])	Train an EmbeddingModel (with optional early stopping).
get_embeddings(entities[, embedding_type])	Get the embeddings of entities or relations.
predict(X[, from_idx, get_ranks])	Predict the scores of triples using a trained embedding model.
_fn(e_s, e_p, e_o)	The scoring function of the model.
_initialize_parameters()	Initialize parameters of the model.
_get_model_loss(dataset_iterator)	Get the current loss including loss due to regularization.
get_embedding_model_params(output_dict)	save the model parameters in the dictionary.
restore_model_params(in_dict)	Load the model parameters from the input dictionary.
_save_trained_params()	After model fitting, save all the trained parameters in trained_model_params in some order.
_load_model_from_trained_params()	Load the model from trained params.
_initialize_early_stopping()	Initializes and creates evaluation graph for early stopping
_perform_early_stopping_test(epoch)	perform regular validation checks and stop early if the criteria is acheived :param epoch: current training epoch :type epoch: int
configure_evaluation_protocol([config])	Set the configuration for evaluation
set_filter_for_eval(x_filter)	Set the filter to be used during evaluation (filtered_corruption = corruptions - filter).
_initialize_eval_graph()	Initialize the evaluation graph.
end_evaluation()	End the evaluation and close the Tensorflow session.

`__init__`(*k=100*, *eta=2*, *epochs=100*, *batches_count=100*, *seed=0*, *embedding_model_params={}*, *optimizer='adam'*, *optimizer_params={'lr': 0.0005}*, *loss='nll'*, *loss_params={}*, *regularizer=None*, *regularizer_params={}*, *verbose=False*)

Initialize an EmbeddingModel

Also creates a new Tensorflow session for training.

Parameters

- **k** (*int*) – Embedding space dimensionality
- **eta** (*int*) – The number of negatives that must be generated at runtime during training for each positive.
- **epochs** (*int*) – The iterations of the training loop.
- **batches_count** (*int*) – The number of batches in which the training set must be split during the training loop.
- **seed** (*int*) – The seed used by the internal random numbers generator.
- **embedding_model_params** (*dict*) – Model-specific hyperparams, passed to the model as a dictionary. Refer to model-specific documentation for details.
- **optimizer** (*string*) – The optimizer used to minimize the loss function. Choose between 'sgd', 'adagrad', 'adam', 'momentum'.
- **optimizer_params** (*dict*) – Arguments specific to the optimizer, passed as a dictionary.

  Supported keys:

  - **'lr'** (float): learning rate (used by all the optimizers). Default: 0.1.
  - **'momentum'** (float): learning momentum (only used when `optimizer=momentum`). Default: 0.9.

  Example: `optimizer_params={'lr': 0.01}`
- **loss** (*string*) – The type of loss function to use during training.
  - `pairwise` the model will use pairwise margin-based loss function.
  - `nll` the model will use negative loss likelihood.
  - `absolute_margin` the model will use absolute margin likelihood.
  - `self_adversarial` the model will use adversarial sampling loss function.
  - `multiclass_nll` the model will use multiclass nll loss. Switch to multiclass loss defined in [aC15] by passing 'corrupt_sides' as ['s','o'] to embedding_model_params. To use loss defined in [KBK17] pass 'corrupt_sides' as 'o' to embedding_model_params
- **loss_params** (*dict*) – Dictionary of loss-specific hyperparameters. See *loss functions* documentation for additional details.

  Example: `optimizer_params={'lr': 0.01}` if `loss='pairwise'`.
- **regularizer** (*string*) – The regularization strategy to use with the loss function.
  - `None`: the model will not use any regularizer (default)
  - 'LP': the model will use L1, L2 or L3 based on the value of `regularizer_params['p']` (see below).

- **regularizer_params** (*dict*) – Dictionary of regularizer-specific hyperparameters. See the *regularizers* documentation for additional details.

  Example: `regularizer_params={'lambda': 1e-5, 'p': 2}` if `regularizer='LP'`.

- **verbose** (*bool*) – Verbose mode

fit (*X*, *early_stopping=False*, *early_stopping_params={}*)
Train an EmbeddingModel (with optional early stopping).

The model is trained on a training set X using the training protocol described in [TWR+16].

Parameters

- **X** (*ndarray, shape [n, 3]*) – The training triples
- **early_stopping** (*bool*) – Flag to enable early stopping (default:`False`)
- **early_stopping_params** (*dictionary*) – Dictionary of hyperparameters for the early stopping heuristics.

  The following string keys are supported:

  - **'x_valid'**: ndarray, shape [n, 3] : Validation set to be used for early stopping.
  - **'criteria'**: string : criteria for early stopping 'hits10', 'hits3', 'hits1' or 'mrr'(default).
  - **'x_filter': ndarray, shape [n, 3]** [Positive triples to use as filter if a 'filtered' early] stopping criteria is desired (i.e. filtered-MRR if 'criteria':'mrr'). Note this will affect training time (no filter by default).
  - **'burn_in'**: int : Number of epochs to pass before kicking in early stopping (default: 100).
  - **check_interval'**: int : Early stopping interval after burn-in (default:10).
  - **'stop_interval'**: int : Stop if criteria is performing worse over n consecutive checks (default: 3)
  - **'corruption_entities': List of entities to be used for corruptions. If 'all',** it uses all entities (default: 'all')
  - **'corrupt_side'**: Specifies which side to corrupt. 's', 'o', 's+o' (default)

  Example: `early_stopping_params={x_valid=X['valid'], 'criteria': 'mrr'}`

get_embeddings (*entities*, *embedding_type='entity'*)
Get the embeddings of entities or relations.

Parameters

- **entities** (*array-like, dtype=int, shape=[n]*) – The entities (or relations) of interest. Element of the vector must be the original string literals, and not internal IDs.
- **embedding_type** (*string*) – If 'entity', the `entities` argument will be considered as a list of knowledge graph entities (i.e. nodes). If set to 'relation', they will be treated as relation types instead (i.e. predicates).

Returns embeddings – An array of k-dimensional embeddings.

Return type ndarray, shape [n, k]

predict (*X*, *from_idx=False*, *get_ranks=False*)
Predict the scores of triples using a trained embedding model.

The function returns raw scores generated by the model.

Note: To obtain probability estimates, use a logistic sigmoid:

```
>>> model.fit(X)
>>> y_pred = model.predict(np.array([['f', 'y', 'e'], ['b', 'y', 'd
↪']]))
>>> print(y_pred)
array([1.2052395, 1.5818497], dtype=float32)
>>> from scipy.special import expit
>>> expit(y_pred)
array([0.7694556 , 0.82946634], dtype=float32)
```

Parameters

- **X** (*ndarray, shape [n, 3]*) – The triples to score.
- **from_idx** (*bool*) – If True, will skip conversion to internal IDs. (default: False).
- **get_ranks** (*bool*) – Flag to compute ranks by scoring against corruptions (default: False).

Returns

- **scores_predict** (*ndarray, shape [n]*) – The predicted scores for input triples X.
- **rank** (*ndarray, shape [n]*) – Ranks of the triples (only returned if `get_ranks=True`.

_fn (*e_s*, *e_p*, *e_o*)
The scoring function of the model.

Assigns a score to a list of triples, with a model-specific strategy. Triples are passed as lists of subject, predicate, object embeddings. This function must be overridden by every model to return corresponding score.

Parameters

- **e_s** (*Tensor, shape [n]*) – The embeddings of a list of subjects.
- **e_p** (*Tensor, shape [n]*) – The embeddings of a list of predicates.
- **e_o** (*Tensor, shape [n]*) – The embeddings of a list of objects.

Returns **score** – The operation corresponding to the scoring function.

Return type TensorFlow operation

_initialize_parameters ()
Initialize parameters of the model.

This function creates and initializes entity and relation embeddings (with size k). Overload this function if the parameters needs to be initialized differently.

_get_model_loss (*dataset_iterator*)

Get the current loss including loss due to regularization. This function must be overridden if the model uses combination of different losses(eg: VAE)

Parameters **dataset_iterator** (*tf.data.Iterator*) – Dataset iterator

Returns **loss** – The loss value that must be minimized.

Return type tf.Tensor

get_embedding_model_params(*output_dict*)
save the model parameters in the dictionary.

Parameters **output_dict** (*dictionary*) – Dictionary of saved params. It's the duty of the model to save all the variables correctly, so that it can be used for restoring later.

restore_model_params(*in_dict*)
Load the model parameters from the input dictionary.

Parameters **in_dict** (*dictionary*) – Dictionary of saved params. It's the duty of the model to load the variables correctly

_save_trained_params()
After model fitting, save all the trained parameters in trained_model_params in some order. The order would be useful for loading the model. This method must be overridden if the model has any other parameters (apart from entity-relation embeddings)

_load_model_from_trained_params()
Load the model from trained params. While restoring make sure that the order of loaded parameters match the saved order. It's the duty of the embedding model to load the variables correctly. This method must be overridden if the model has any other parameters (apart from entity-relation embeddings)

_initialize_early_stopping()
Initializes and creates evaluation graph for early stopping

_perform_early_stopping_test(*epoch*)
perform regular validation checks and stop early if the criteria is acheived :param epoch: current training epoch :type epoch: int

Returns **stopped** – Flag to indicate if the early stopping criteria is acheived

Return type bool

configure_evaluation_protocol(*config={'corrupt_side': 's+o', 'corruption_entities': 'all', 'default_protocol': False}*)
Set the configuration for evaluation

Parameters **config** (*dictionary*) – Dictionary of parameters for evaluation configuration. Can contain following keys:

- **corruption_entities**: List of entities to be used for corruptions. If `all`, it uses all entities (default: `all`)
- **corrupt_side**: Specifies which side to corrupt. `s`, `o`, `s+o` (default)
- **default_protocol**: Boolean flag to indicate whether to use default protocol for evaluation. This computes scores for corruptions of subjects and objects and ranks them separately. This could have been done by evaluating s and o separately and then ranking but it slows down the performance. Hence this mode is used where s+o corruptions are generated at once but ranked separately for speed up.(default: False)

set_filter_for_eval (*x_filter*)

Set the filter to be used during evaluation (filtered_corruption = corruptions - filter).

We would be using a prime number based assignment and product for do the filtering. We associate a unique prime number for subject entities, object entities and to relations. Product of three prime numbers is divisible only by those three prime numbers. So we generate this product for the filter triples and store it in a hash map. When corruptions are generated for a triple during evaluation, we follow a similar approach and look up the product of corruption in the above hash table. If the corrupted triple is present in the hashmap, it means that it was present in the filter list.

Parameters **x_filter** (*ndarray, shape [n, 3]*) – Filter triples. If the generated corruptions are present in this, they will be removed.

_initialize_eval_graph ()

Initialize the evaluation graph.

Use prime number based filtering strategy (refer set_filter_for_eval()), if the filter is set

end_evaluation ()

End the evaluation and close the Tensorflow session.

Loss

class ampligraph.latent_features.**Loss** (*eta*, *hyperparam_dict*, *verbose=False*)

Abstract class for loss function.

Methods

__init__(eta, hyperparam_dict[, verbose])	Initialize Loss.
get_state(param_name)	Get the state value.
_init_hyperparams(hyperparam_dict)	Initializes the hyperparameters needed by the algorithm.
_inputs_check(scores_pos, scores_neg)	Creates any dependencies that need to be checked before performing loss computations
apply(scores_pos, scores_neg)	Interface to external world.
_apply(scores_pos, scores_neg)	Apply the loss function.

__init__ (*eta*, *hyperparam_dict*, *verbose=False*)

Initialize Loss.

Parameters

- **eta** (*int*) – number of negatives
- **hyperparam_dict** (*dict*) – dictionary of hyperparams. (Keys are described in the hyperparameters section)

get_state (*param_name*)

Get the state value.

Parameters **param_name** (*string*) – name of the state for which one wants to query the value

Returns the value of the corresponding state

Return type param_value

_init_hyperparams (*hyperparam_dict*)
Initializes the hyperparameters needed by the algorithm.

Parameters **hyperparam_dict** (*dictionary*) – Consists of key value pairs. The Loss will check the keys to get the corresponding params

_inputs_check (*scores_pos*, *scores_neg*)
Creates any dependencies that need to be checked before performing loss computations

Parameters

- **scores_pos** (*tf.Tensor*) – A tensor of scores assigned to positive statements.
- **scores_neg** (*tf.Tensor*) – A tensor of scores assigned to negative statements.

apply (*scores_pos*, *scores_neg*)
Interface to external world. This function does the input checks, preprocesses input and finally applies loss function.

Parameters

- **scores_pos** (*tf.Tensor*) – A tensor of scores assigned to positive statements.
- **scores_neg** (*tf.Tensor*) – A tensor of scores assigned to negative statements.

Returns **loss** – The loss value that must be minimized.

Return type tf.Tensor

_apply (*scores_pos*, *scores_neg*)
Apply the loss function. Every inherited class must implement this function. (All the TF code must go in this function.)

Parameters

- **scores_pos** (*tf.Tensor*) – A tensor of scores assigned to positive statements.
- **scores_neg** (*tf.Tensor*) – A tensor of scores assigned to negative statements.

Returns **loss** – The loss value that must be minimized.

Return type tf.Tensor

Regularizer

class ampligraph.latent_features.**Regularizer** (*hyperparam_dict*, *verbose=False*)
Abstract class for Regularizer.

Methods

__init__(hyperparam_dict[, verbose])	Initialize the regularizer.
get_state(param_name)	Get the state value.
_init_hyperparams(hyperparam_dict)	Initializes the hyperparameters needed by the algorithm.
apply(trainable_params)	Interface to external world.
_apply(trainable_params)	Apply the regularization function.

`__init__`(*hyperparam_dict*, *verbose=False*)
Initialize the regularizer.

Parameters **hyperparam_dict** (`dict`) – dictionary of hyperparams (Keys are described in the hyperparameters section)

`get_state`(*param_name*)
Get the state value.

Parameters **param_name** (`string`) – name of the state for which one wants to query the value

Returns the value of the corresponding state

Return type param_value

`_init_hyperparams`(*hyperparam_dict*)
Initializes the hyperparameters needed by the algorithm.

Parameters **hyperparam_dict** (`dictionary`) – Consists of key value pairs. The regularizer will check the keys to get the corresponding params

`apply`(*trainable_params*)
Interface to external world. This function performs input checks, input pre-processing, and and applies the loss function.

Parameters **trainable_params** (`list, shape [n]`) – List of trainable params that should be reqularized

Returns **loss** – Regularization Loss

Return type tf.Tensor

`_apply`(*trainable_params*)
Apply the regularization function. Every inherited class must implement this function.

(All the TF code must go in this function.)

Parameters **trainable_params** (`list, shape [n]`) – List of trainable params that should be reqularized

Returns **loss** – Regularization Loss

Return type tf.Tensor

Scoring functions

Existing models propose scoring functions that combine the embeddings $\mathbf{e}_s, \mathbf{r}_p, \mathbf{e}_o \in \mathcal{R}^k$ of the subject, predicate, and object of a triple $t = (s, p, o)$ according to different intuitions:

- `TransE` [BUGD+13] relies on distances. The scoring function computes a similarity between the embedding of the subject translated by the embedding of the predicate and the embedding of the object, using the L_1 or L_2 norm $|| \cdot ||$:

$$f_{TransE} = -||\mathbf{e}_s + \mathbf{r}_p - \mathbf{e}_o||_n$$

- `DistMult` [YYH+14] uses the trilinear dot product:

$$f_{DistMult} = \langle \mathbf{r}_p, \mathbf{e}_s, \mathbf{e}_o \rangle$$

- `ComplEx` [TWR+16] extends DistMult with the Hermitian dot product:

$$f_{ComplEx} = Re(\langle \mathbf{r}_p, \mathbf{e}_s, \overline{\mathbf{e}_o} \rangle)$$

- *HolE* [NRP+16] uses circular correlation.

$$f_{HolE} = \mathbf{w}_r \cdot (\mathbf{e}_s \star \mathbf{e}_o) = \frac{1}{k}\mathcal{F}(\mathbf{w}_r) \cdot (\overline{\mathcal{F}(\mathbf{e}_s)} \odot \mathcal{F}(\mathbf{e}_o))$$

Other models such ConvE include convolutional layers [DMSR18] (will be available in AmpliGraph future releases).

Loss Functions

AmpliGraph includes a number of loss functions commonly used in literature. Each function can be used with any of the implemented models. Loss functions are passed to models as hyperparameter, and they can be thus used *during model selection*.

`PairwiseLoss`(eta[, loss_params, verbose])	Pairwise, max-margin loss.
`AbsoluteMarginLoss`(eta[, loss_params, verbose])	Absolute margin , max-margin loss.
`SelfAdversarialLoss`(eta[, loss_params, verbose])	Self adversarial sampling loss.
`NLLLoss`(eta[, loss_params, verbose])	Negative log-likelihood loss.
`NLLMulticlass`(eta[, loss_params, verbose])	Multiclass NLL Loss.

PairwiseLoss

class ampligraph.latent_features.**PairwiseLoss**(*eta*, *loss_params={'margin': 1}*, *verbose=False*)

Pairwise, max-margin loss.

Introduced in [BUGD+13].

$$\mathcal{L}(\Theta) = \sum_{t^+ \in \mathcal{G}} \sum_{t^- \in \mathcal{C}} max(0, [\gamma + f_{model}(t^-;\Theta) - f_{model}(t^+;\Theta)])$$

where γ is the margin, $\mathcal{G}$ is the set of positives, $\mathcal{C}$ is the set of corruptions, $f_{model}(t;\Theta)$ is the model-specific scoring function.

Methods

`__init__`(eta[, loss_params, verbose])	Initialize Loss.

__init__(*eta*, *loss_params={'margin': 1}*, *verbose=False*)

Initialize Loss.

Parameters

- **eta** (*int*) – number of negatives
- **loss_params** (*dict*) – Dictionary of loss-specific hyperparams:
  - **'margin'**: (float). Margin to be used in pairwise loss computation (default: 1)

  Example: `loss_params={'margin': 1}`

AbsoluteMarginLoss

class ampligraph.latent_features.**AbsoluteMarginLoss**(*eta*, *loss_params={'margin': 1}*, *verbose=False*)

Absolute margin , max-margin loss.

Introduced in [HOSM17].

$$\mathcal{L}(\Theta) = \sum_{t^+ \in \mathcal{G}}\sum_{t^- \in \mathcal{C}} f_{model}(t^-;\Theta) - max(0, [\gamma - f_{model}(t^+;\Theta)])$$

where γ is the margin, $\mathcal{G}$ is the set of positives, $\mathcal{C}$ is the set of corruptions, $f_{model}(t;\Theta)$ is the model-specific scoring function.

Methods

`__init__`(eta[, loss_params, verbose])	Initialize Loss

__init__(*eta*, *loss_params={'margin': 1}*, *verbose=False*)

Initialize Loss

Parameters

- **eta** (*int*) – number of negatives
- **loss_params** (*dict*) – Dictionary of loss-specific hyperparams:
  - **'margin'**: float. Margin to be used in pairwise loss computation (default:1)

  Example: `loss_params={'margin': 1}`

SelfAdversarialLoss

class ampligraph.latent_features.**SelfAdversarialLoss**(*eta*, *loss_params={'alpha': 0.5, 'margin': 3}*, *verbose=False*)

Self adversarial sampling loss.

Introduced in [SDNT19].

$$\mathcal{L} = -log\, \sigma(\gamma + f_{model}(\mathbf{s},\mathbf{o})) - \sum_{i=1}^{n} p(h_{i}^{'}, r, t_{i}^{'})\ log\ \sigma(-f_{model}(\mathbf{s}_{i}^{'},\mathbf{o}_{i}^{'}) - \gamma)$$

where $\mathbf{s}, \mathbf{o} \in \mathcal{R}^k$ are the embeddings of the subject and object of a triple $t = (s, r, o)$, γ is the margin, σ the sigmoid function, and $p(s_{i}^{'}, r, o_{i}^{'})$ is the negatives sampling distribution which is defined as:

$$p(s'_j, r, o'_j | \{(s_i, r_i, o_i)\}) = \frac{\exp \alpha\, f_{model}(\mathbf{s'_j}, \mathbf{o'_j})}{\sum_i \exp \alpha\, f_{model}(\mathbf{s'_i}, \mathbf{o'_i})}$$

where α is the temperature of sampling, f_{model} is the scoring function of the desired embeddings model.

Methods

`__init__`(eta[, loss_params, verbose])	Initialize Loss

__init__(*eta*, *loss_params={'alpha': 0.5, 'margin': 3}*, *verbose=False*)

Initialize Loss

Parameters

- **eta** (*int*) – number of negatives
- **loss_params** (*dict*) – Dictionary of loss-specific hyperparams:
  - **'margin'**: (float). Margin to be used for loss computation (default: 1)
  - **'alpha'** : (float). Temperature of sampling (default:0.5)

  Example: `loss_params={'margin': 1, 'alpha': 0.5}`

NLLLoss

class ampligraph.latent_features.**NLLLoss**(*eta*, *loss_params={}*, *verbose=False*)

Negative log-likelihood loss.

As described in [TWR+16].

$$\mathcal{L}(\Theta) = \sum_{t \in \mathcal{G} \cup \mathcal{C}} log(1 + exp(-y \, f_{model}(t;\Theta)))$$

where $y \in -1, 1$ is the label of the statement, $\mathcal{G}$ is the set of positives, $\mathcal{C}$ is the set of corruptions, $f_{model}(t;\Theta)$ is the model-specific scoring function.

Methods

`__init__`(eta[, loss_params, verbose])	Initialize Loss.

__init__(*eta*, *loss_params={}*, *verbose=False*)

Initialize Loss.

Parameters

- **eta** (*int*) – number of negatives
- **loss_params** (*dict*) – dictionary of hyperparams. No hyperparameters are required for this loss.

NLLMulticlass

class ampligraph.latent_features.**NLLMulticlass**(*eta*, *loss_params={}*, *verbose=False*)

Multiclass NLL Loss.

Introduced in [aC15] where both the subject and objects are corrupted (to use it in this way pass corrupt_sides = ['s', 'o'] to embedding_model_params) .

This loss was re-engineered in [KBK17] where only the object was corrupted to get improved performance (to use it in this way pass corrupt_sides = 'o' to embedding_model_params).

$$\mathcal{L}(\mathcal{X}) = -\sum_{x_{e_1,e_2,r_k} \in X} log\,p(e_2|e_1,r_k) - \sum_{x_{e_1,e_2,r_k} \in X} log\,p(e_1|r_k, e_2)$$

Examples

```
>>> from ampligraph.latent_features import TransE
>>> model = TransE(batches_count=1, seed=555, epochs=20, k=10,
>>>                embedding_model_params={'corrupt_sides':['s', 'o']},
>>>                loss='multiclass_nll', loss_params={})
```

Methods

__init__(eta[, loss_params, verbose])	Initialize Loss

__init__(*eta*, *loss_params={}*, *verbose=False*)
Initialize Loss

Parameters

- **eta** (*int*) – number of negatives
- **loss_params** (*dict*) – Dictionary of loss-specific hyperparams:

Regularizers

AmpliGraph includes a number of regularizers that can be used with the *loss function*. *LPRegularizer* supports L1, L2, and L3.

LPRegularizer([regularizer_params, verbose])	Performs LP regularization

LPRegularizer

class ampligraph.latent_features.**LPRegularizer**(*regularizer_params={'lambda': 1e-05, 'p': 2}*, *verbose=False*)
Performs LP regularization

$$\mathcal{L}(Reg) = \sum_{i=1}^{n} \lambda_i * \mid w_i \mid_p$$

where n is the number of model parameters, $p \in 1, 2, 3$ is the p-norm and λ is the regularization weight.

Example: if $p = 1$ the function will perform L1 regularization. L2 regularization is obtained with $p = 2$.

Methods

__init__([regularizer_params, verbose])	Initializes the hyperparameters needed by the algorithm.

__init__(*regularizer_params={'lambda': 1e-05, 'p': 2}*, *verbose=False*)
Initializes the hyperparameters needed by the algorithm.

Parameters **regularizer_params** (*dictionary*) – Consists of key-value pairs. The regularizer will check the keys to get the corresponding params:

- **'lambda'**: (float). Weight of regularization loss for each parameter (default: 1e-5)
- **'p'**: (int): norm (default: 2)

Example: `regularizer_params={'lambda': 1e-5, 'p': 1}`

Optimizers

The goal of the optimization procedure is learning optimal embeddings, such that the scoring function is able to assign high scores to positive statements and low scores to statements unlikely to be true.

We support SGD-based optimizers provided by TensorFlow, by setting the `optimizer` argument in a model initializer. Best results are currently obtained with Adam.

Saving/Restoring Models

Models can be saved and restored from disk. This is useful to avoid re-training a model.

More details in the *utils* module.

3.3.3 Evaluation

The module includes performance metrics for neural graph embeddings models, along with model selection routines, negatives generation, and an implementation of the learning-to-rank-based evaluation protocol used in literature.

Metrics

Learning-to-rank metrics to evaluate the performance of neural graph embedding models.

rank_score(y_true, y_pred[, pos_lab])	Rank of a triple
mrr_score(ranks)	Mean Reciprocal Rank (MRR)
mr_score(ranks)	Mean Rank (MR)
hits_at_n_score(ranks, n)	Hits@N

rank_score

`ampligraph.evaluation.`**`rank_score`**(*y_true*, *y_pred*, *pos_lab=1*)

Rank of a triple

The rank of a positive element against a list of negatives.

$$rank_{(s,p,o)_i}$$

Parameters

- **y_true** (*ndarray, shape [n]*) – An array of binary labels. The array only contains one positive.
- **y_pred** (*ndarray, shape [n]*) – An array of scores, for the positive element and the n-1 negatives.
- **pos_lab** (*int*) – The value of the positive label (default = 1)

Returns **rank** – The rank of the positive element against the negatives.

Return type int

Examples

```
>>> import numpy as np
>>> from ampligraph.evaluation.metrics import rank_score
>>> y_pred = np.array([.434, .65, .21, .84])
>>> y_true = np.array([0, 0, 1, 0])
>>> rank_score(y_true, y_pred)
4
```

mrr_score

`ampligraph.evaluation.mrr_score(ranks)`

Mean Reciprocal Rank (MRR)

The function computes the mean of the reciprocal of elements of a vector of rankings `ranks`.

It is used in conjunction with the learning to rank evaluation protocol of *ampligraph.evaluation.evaluate_performance()*.

It is formally defined as follows:

$$MRR = \frac{1}{|Q|}\sum_{i = 1}^{|Q|}\frac{1}{rank_{(s, p, o)_i}}$$

where Q is a set of triples and (s, p, o) is a triple $\in Q$.

Note: This metric is similar to mean rank (MR) *ampligraph.evaluation.mr_score()*. Instead of averaging ranks, it averages their reciprocals. This is done to obtain a metric which is more robust to outliers.

Consider the following example. Each of the two positive triples identified by * are ranked against four corruptions each. When scored by an embedding model, the first triple ranks 2nd, and the other triple ranks first. The resulting MRR is:

```
s        p         o            score   rank
Jack   born_in   Ireland        0.789      1
Jack   born_in   Italy          0.753      2    *
Jack   born_in   Germany        0.695      3
Jack   born_in   China          0.456      4
Jack   born_in   Thomas         0.234      5

s        p         o            score   rank
Jack   friend_with   Thomas     0.901      1    *
Jack   friend_with   China      0.345      2
Jack   friend_with   Italy      0.293      3
Jack   friend_with   Ireland    0.201      4
Jack   friend_with   Germany    0.156      5

MRR=0.75
```

Parameters **ranks** (*ndarray, shape [n]*) – Input ranks of n positive statements.

Returns **hits_n_score** – The MRR score

Return type float

Examples

```
>>> import numpy as np
>>> from ampligraph.evaluation.metrics import mrr_score
>>> rankings = np.array([1, 12, 6, 2])
>>> mrr_score(rankings)
0.4375
```

mr_score

ampligraph.evaluation.**mr_score**(*ranks*)

Mean Rank (MR)

The function computes the mean of of a vector of rankings `ranks`.

It can be used in conjunction with the learning to rank evaluation protocol of *ampligraph.evaluation.evaluate_performance()*.

It is formally defined as follows:

$$MR = \frac{1}{|Q|}\sum_{i=1}^{|Q|} rank_{(s,p,o)_i}$$

where Q is a set of triples and (s, p, o) is a triple $\in Q$.

Note: This metric is not robust to outliers. It is usually presented along the more reliable MRR *ampligraph.evaluation.mrr_score()*.

Consider the following example. Each of the two positive triples identified by $*$ are ranked against four corruptions each. When scored by an embedding model, the first triple ranks 2nd, and the other triple ranks first. The resulting MR is:

```
s        p         o            score   rank
Jack   born_in   Ireland        0.789      1
Jack   born_in   Italy          0.753      2   *
Jack   born_in   Germany        0.695      3
Jack   born_in   China          0.456      4
Jack   born_in   Thomas         0.234      5

s        p         o            score   rank
Jack   friend_with   Thomas     0.901      1   *
Jack   friend_with   China      0.345      2
Jack   friend_with   Italy      0.293      3
Jack   friend_with   Ireland    0.201      4
Jack   friend_with   Germany    0.156      5

MR=1.5
```

Examples

```
>>> from ampligraph.evaluation import mr_score
>>> ranks= [5, 3, 4, 10, 1]
```

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```
>>> mr_score(ranks)
4.6
```

hits_at_n_score

ampligraph.evaluation.**hits_at_n_score**(*ranks*, *n*)

Hits@N

The function computes how many elements of a vector of rankings `ranks` make it to the top `n` positions.

It can be used in conjunction with the learning to rank evaluation protocol of `ampligraph.evaluation.evaluate_performance()`.

It is formally defined as follows:

$$Hits@N = \sum_{i=1}^{|Q|} 1 \, if rank_{(s,p,o)_i} \leq N$$

where Q is a set of triples and (s, p, o) is a triple $\in Q$.

Consider the following example. Each of the two positive triples identified by * are ranked against four corruptions each. When scored by an embedding model, the first triple ranks 2nd, and the other triple ranks first. Hits@1 and Hits@3 are:

```
s        p         o            score   rank
Jack   born_in   Ireland        0.789      1
Jack   born_in   Italy          0.753      2    *
Jack   born_in   Germany        0.695      3
Jack   born_in   China          0.456      4
Jack   born_in   Thomas         0.234      5

s        p         o            score   rank
Jack   friend_with   Thomas     0.901      1    *
Jack   friend_with   China      0.345      2
Jack   friend_with   Italy      0.293      3
Jack   friend_with   Ireland    0.201      4
Jack   friend_with   Germany    0.156      5

Hits@3=1.0
Hits@1=0.5
```

Parameters

- **ranks** (*ndarray, shape [n]*) – Input ranks of n positive statements.
- **n** (*int*) – The maximum rank considered to accept a positive.

Returns **hits_n_score** – The Hits@n score

Return type float

Examples

```
>>> import numpy as np
>>> from ampligraph.evaluation.metrics import hits_at_n_score
>>> rankings = np.array([1, 12, 6, 2])
>>> hits_at_n_score(rankings, n=3)
0.5
```

Negatives Generation

Negatives generation routines. These are corruption strategies based on the Local Closed-World Assumption (LCWA).

generate_corruptions_for_eval(X, ...[, ...])	Generate corruptions for evaluation.
generate_corruptions_for_fit(X[, ...])	Generate corruptions for training.

generate_corruptions_for_eval

ampligraph.evaluation.**generate_corruptions_for_eval**(*X*, *entities_for_corruption*, *corrupt_side='s+o'*, *table_entity_lookup_left=None*, *table_entity_lookup_right=None*, *table_reln_lookup=None*)

Generate corruptions for evaluation.

Create corruptions (subject and object) for a given triple x, in compliance with the local closed world assumption (LCWA), as described in [NMTG16].

Note: For filtering the corruptions, we adopt a hashing-based strategy to handle the set difference problem. This strategy is as described below:

- We compute unique entities and relations in our dataset.
- We assign unique prime numbers for entities (unique for subject and object separately) and for relations and create three separate hash tables. (these hash maps are input to this function)
- For each triple in filter_triples, we get the prime numbers associated with subject, relation and object by mapping to their respective hash tables. We then compute the **prime product for the filter triple**. We store this triple product.
- Since the numbers assigned to subjects, relations and objects are unique, their prime product is also unique. i.e. a triple (a, b, c) would have a different product compared to triple (c, b, a) as a, c of subject have different primes compared to a, c of object.
- While generating corruptions for evaluation, we hash the triple's entities and relations and get the associated prime number and compute the **prime product for the corrupted triple**.
- If this product is present in the products stored for the filter set, then we remove the corresponding corrupted triple (as it is a duplicate i.e. the corruption triple is present in filter_triples)
- Using this approach we generate filtered corruptions for evaluation.

Execution Time: This method takes ~20 minutes on FB15K using ComplEx (Intel Xeon Gold 6142, 64 GB Ubuntu 16.04 box, Tesla V100 16GB)

Parameters

- **X** (*Tensor, shape [1, 3]*) – Currently, a single positive triples that will be used to create corruptions.
- **entities_for_corruption** (*Tensor*) – All the entity IDs which are to be used for generation of corruptions
- **corrupt_side** (*string*) – Specifies which side of the triple to corrupt:
  - 's': corrupt only subject.
  - 'o': corrupt only object
  - 's+o': corrupt both subject and object
- **table_entity_lookup_left** (*tf.HashTable*) – Hash table of subject entities mapped to unique prime numbers
- **table_entity_lookup_right** (*tf.HashTable*) – Hash table of object entities mapped to unique prime numbers
- **table_reln_lookup** (*tf.HashTable*) – Hash table of relations mapped to unique prime numbers

Returns

- **out** (*Tensor, shape [n, 3]*) – An array of corruptions for the triples for x.
- **out_prime** (*Tensor, shape [n, 3]*) – An array of product of prime numbers associated with corruption triples or None based on filtered or non filtered version.

generate_corruptions_for_fit

`ampligraph.evaluation.generate_corruptions_for_fit(X, entities_list=None, eta=1, corrupt_side='s+o', entities_size=0, rnd=None)`

Generate corruptions for training.

Creates corrupted triples for each statement in an array of statements, as described by [TWR+16].

Note: Collisions are not checked, as this will be computationally expensive [TWR+16]. That means that some corruptions *may* result in being positive statements (i.e. *unfiltered* settings).

Note: When processing large knowledge graphs, it may be useful to generate corruptions only using entities from a single batch. This also brings the benefit of creating more meaningful negatives, as entities used to corrupt are sourced locally. The function can be configured to generate corruptions *only* using the entities from the current batch. You can enable such behaviour be setting `entities_size==-1`. In such case, if `entities_list=None` all entities from the *current batch* will be used to generate corruptions.

Parameters

- **X** (*Tensor, shape [n, 3]*) – An array of positive triples that will be used to create corruptions.
- **entities_list** (*list*) – List of entities to be used for generating corruptions. (default:None). if `entities_list=None`, all entities will be used to generate corruptions (default behaviour).

- **eta** (*int*) – The number of corruptions per triple that must be generated.
- **corrupt_side** (*string*) – Specifies which side of the triple to corrupt:
  - 's': corrupt only subject.
  - 'o': corrupt only object
  - 's+o': corrupt both subject and object
- **entities_size** (*int*) – Size of entities to be used while generating corruptions. It assumes entity id's start from 0 and are continuous. (default: 0). When processing large knowledge graphs, it may be useful to generate corruptions only using entities from a single batch. This also brings the benefit of creating more meaningful negatives, as entities used to corrupt are sourced locally. The function can be configured to generate corruptions *only* using the entities from the current batch. You can enable such behaviour be setting `entities_size==-1`. In such case, if `entities_list=None` all entities from the *current batch* will be used to generate corruptions.
- **rnd** (*numpy.random.RandomState*) – A random number generator.

Returns **out** – An array of corruptions for a list of positive triples x. For each row in X the corresponding corruption indexes can be found at [index+i*n for i in range(eta)]

Return type Tensor, shape [n * eta, 3]

Evaluation & Model Selection

Functions to evaluate the predictive power of knowledge graph embedding models, and routines for model selection.

evaluate_performance(X, model[, ...])	Evaluate the performance of an embedding model.
select_best_model_ranking(model_class, X, ...)	Model selection routine for embedding models.

evaluate_performance

ampligraph.evaluation.**evaluate_performance**(*X*, *model*, *filter_triples=None*, *verbose=False*, *strict=True*, *rank_against_ent=None*, *corrupt_side='s+o'*, *use_default_protocol=True*)

Evaluate the performance of an embedding model.

Run the relational learning evaluation protocol defined in [BUGD+13].

It computes the rank of each positive triple against a number of negatives generated on the fly. Such negatives are compliant with the local closed world assumption (LCWA), as described in [NMTG16]. In practice, that means only one side of the triple is corrupted (i.e. either the subject or the object).

Note: When *filtered* mode is enabled (i.e. *filtered_triples* is not `None`), to speed up the procedure, we adopt a hashing-based strategy to handle the set difference problem. This strategy is as described below:

- We compute unique entities and relations in our dataset.
- We assign unique prime numbers for entities (unique for subject and object separately) and for relations and create three separate hash tables.
- For each triple in `filter_triples`, we get the prime numbers associated with subject,

relation and object by mapping to their respective hash tables. We then compute the **prime product for the filter triple**. We store this triple product.

- Since the numbers assigned to subjects, relations and objects are unique, their prime product is also unique. i.e. a triple (a, b, c) would have a different product compared to triple (c, b, a) as a, c of subject have different primes compared to a, c of object.
- While generating corruptions for evaluation, we hash the triple's entities and relations and get the associated prime number and compute the **prime product for the corrupted triple**.
- If this product is present in the products stored for the filter set, then we remove the corresponding corrupted triple (as it is a duplicate i.e. the corruption triple is present in `filter_triples`)
- Using this approach we generate filtered corruptions for evaluation.

Execution Time: This method takes ~20 minutes on FB15K using ComplEx (Intel Xeon Gold 6142, 64 GB Ubuntu 16.04 box, Tesla V100 16GB)

Hint: When `rank_against_ent=None`, the method will use all distinct entities in the knowledge graph `X` to generate negatives to rank against. If `X` includes more than 1 million unique entities and relations, the method will return a runtime error. To solve the problem, it is recommended to pass the desired entities to use to generate corruptions to `rank_against_ent`. Besides, trying to rank a positive against an extremely large number of negatives may be overkilling. As a reference, the popular FB15k-237 dataset has ~15k distinct entities. The evaluation protocol ranks each positives against 15k corruptions per side.

Parameters

- **X** (*ndarray, shape [n, 3]*) – An array of test triples.
- **model** (EmbeddingModel) – A knowledge graph embedding model
- **filter_triples** (*ndarray of shape [n, 3] or None*) – The triples used to filter negatives.
- **verbose** (*bool*) – Verbose mode
- **strict** (*bool*) – Strict mode. If True then any unseen entity will cause a RuntimeError. If False then triples containing unseen entities will be filtered out.
- **rank_against_ent** (*array-like*) – List of entities to use for corruptions. If None, will generate corruptions using all distinct entities. Default is None.
- **corrupt_side** (*string*) – Specifies which side of the triple to corrupt:
  - 's': corrupt only subject.
  - 'o': corrupt only object
  - 's+o': corrupt both subject and object. The same behaviour is obtained with `use_default_protocol=True`.

Note: If `corrupt_side='s+o'` the function will return 2*n ranks. If `corrupt_side='s'` or `corrupt_side='o'`, it will return n ranks, where n is the number of statements in X. The first n elements of ranks are obtained against subject corruptions. From n+1 until 2n ranks are obtained against object corruptions.

- **use_default_protocol** (*bool*) – Flag to indicate whether to use the standard protocol used in literature defined in [BUGD+13] (default: True). If set to `True` it is equivalent to `corrupt_side='s+o'`. This corresponds to the evaluation protcol used in literature, where head and tail corruptions are evaluated separately.

  Note: When `use_default_protocol=True` the function will return 2*n ranks. The first n elements of ranks are obtained against subject corruptions. From n+1 until 2n ranks are obtained against object corruptions.

Returns ranks – An array of ranks of positive test triples. When `use_default_protocol=True` or `corrupt_side='s+o'`, the function returns 2*n ranks instead of n. In that case the first n elements of ranks are obtained against subject corruptions. From n+1 until 2n ranks are obtained against object corruptions.

Return type ndarray, shape [n] or [2*n]

Examples

```
>>> import numpy as np
>>> from ampligraph.datasets import load_wn18
>>> from ampligraph.latent_features import ComplEx
>>> from ampligraph.evaluation import evaluate_performance, mrr_score, hits_at_n_
↪score
>>>
>>> X = load_wn18()
>>> model = ComplEx(batches_count=10, seed=0, epochs=10, k=150, eta=1,
>>>                 loss='nll', optimizer='adam')
>>> model.fit(np.concatenate((X['train'], X['valid'])))
>>>
>>> filter = np.concatenate((X['train'], X['valid'], X['test']))
>>> ranks = evaluate_performance(X['test'][:5], model=model,
                                 filter_triples=filter,
                                 corrupt_side='s+o',
                                 use_default_protocol=False)
>>> ranks
[1, 582, 543, 6, 31]
>>> mrr_score(ranks)
0.24049691297347323
>>> hits_at_n_score(ranks, n=10)
0.4
```

select_best_model_ranking

`ampligraph.evaluation.`**`select_best_model_ranking`**(*model_class*, *X*, *param_grid*, *use_filter=False*, *early_stopping=False*, *early_stopping_params={}*, *use_test_for_selection=True*, *rank_against_ent=None*, *corrupt_side='s+o'*, *use_default_protocol=False*, *verbose=False*)

Model selection routine for embedding models.

Note: By default, model selection is done with raw MRR for better runtime performance (use_filter=False).

The function also retrains the best performing model on the concatenation of training and validation sets.

Note we generate negatives at runtime according to the strategy described in :[BUGD+13]).

Parameters

- **model_class** (*class*) – The class of the EmbeddingModel to evaluate (TransE, DistMult, ComplEx, etc).
- **X** (*dict*) – A dictionary of triples to use in model selection. Must include three keys: *train*, *val*, *test*. Values are ndarray of shape [n, 3]..
- **param_grid** (*dict*) – A grid of hyperparameters to use in model selection. The routine will train a model for each combination of these hyperparameters.
- **use_filter** (*bool*) – If True, will use the entire input dataset X to compute filtered MRR
- **early_stopping** (*bool*) – Flag to enable early stopping (default:False).

  If set to True, the training loop adopts the following early stopping heuristic:

  – The model will be trained regardless of early stopping for burn_in epochs.

  – Every check_interval epochs the method will compute the metric specified in criteria.

  If such metric decreases for stop_interval checks, we stop training early.

  Note the metric is computed on x_valid. This is usually a validation set that you held out.

  Also, because criteria is a ranking metric, it requires generating negatives. Entities used to generate corruptions can be specified, as long as the side(s) of a triple to corrupt. The method supports filtered metrics, by passing an array of positives to x_filter. This will be used to filter the negatives generated on the fly (i.e. the corruptions).

  Note: Keep in mind the early stopping criteria may introduce a certain overhead (caused by the metric computation). The goal is to strike a good trade-off between such overhead and saving training epochs.

  A common approach is to use MRR unfiltered:

```
early_stopping_params={x_valid=X['valid'], 'criteria': 'mrr'}
```

  Note the size of validation set also contributes to such overhead. In most cases a smaller validation set would be enough.

- **early_stopping_params** (*dict*) – Dictionary of parameters for early stopping.

  The following keys are supported:

  x_valid: ndarray, shape [n, 3] : Validation set to be used for early stopping. Uses X['valid'] by default.

criteria: criteria for early stopping hits10, hits3, hits1 or mrr. (default)

x_filter: ndarray, shape [n, 3] : Filter to be used(no filter by default)

burn_in: Number of epochs to pass before kicking in early stopping(default: 100)

check_interval: Early stopping interval after burn-in(default:10)

stop_interval: Stop if criteria is performing worse over n consecutive checks (default: 3)

- **use_test_for_selection** (*bool*) – Use test set for model selection. If False, uses validation set. Default(True)
- **rank_against_ent** (*array-like*) – List of entities to use for corruptions. If None, will generate corruptions using all distinct entities. Default is None.
- **corrupt_side** (*string*) – Specifies which side to corrupt the entities. s is to corrupt only subject. o is to corrupt only object s+o is to corrupt both subject and object
- **use_default_protocol** (*bool*) – Flag to indicate whether to evaluate head and tail corruptions separately(default:False). If this is set to true, it will ignore corrupt_side argument and corrupt both head and tail separately and rank triples.
- **verbose** (*bool*) – Verbose mode during evaluation of trained model

Returns

- **best_model** (*EmbeddingModel*) – The best trained embedding model obtained in model selection.
- **best_params** (*dict*) – The hyperparameters of the best embedding model *best_model*.
- **best_mrr_train** (*float*) – The MRR (unfiltered) of the best model computed over the validation set in the model selection loop.
- **ranks_test** (*ndarray, shape [n]*) – The ranks of each triple in the test set X['test].
- **mrr_test** (*float*) – The MRR (filtered) of the best model, retrained on the concatenation of training and validation sets, computed over the test set.

Examples

```
>>> from ampligraph.datasets import load_wn18
>>> from ampligraph.latent_features import ComplEx
>>> from ampligraph.evaluation import select_best_model_ranking
>>>
>>> X = load_wn18()
>>> model_class = ComplEx
>>> param_grid = {
>>>                     "batches_count": [50],
>>>                     "seed": 0,
>>>                     "epochs": [4000],
>>>                     "k": [100, 200],
>>>                     "eta": [5,10,15],
>>>                     "loss": ["pairwise", "nll"],
>>>                     "loss_params": {
>>>                         "margin": [2]
```

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```
>>>                     },
>>>                     "embedding_model_params": {
>>>
>>>                     },
>>>                     "regularizer": ["LP", None],
>>>                     "regularizer_params": {
>>>                         "p": [1, 3],
>>>                         "lambda": [1e-4, 1e-5]
>>>                     },
>>>                     "optimizer": ["adagrad", "adam"],
>>>                     "optimizer_params":{
>>>                         "lr": [0.01, 0.001, 0.0001]
>>>                     },
>>>                     "verbose": false
>>>                 }
>>> select_best_model_ranking(model_class, X, param_grid, use_filter=True,␣
↪verbose=True, early_stopping=True)
```

Helper Functions

Utilities and support functions for evaluation procedures.

train_test_split_no_unseen(X[, test_size, ...])	Split into train and test sets.
create_mappings(X)	Create string-IDs mappings for entities and relations.
to_idx(X, ent_to_idx, rel_to_idx)	Convert statements (triples) into integer IDs.

train_test_split_no_unseen

`ampligraph.evaluation.`**`train_test_split_no_unseen`**(*X*, *test_size=5000*, *seed=0*, *allow_duplication=False*)

Split into train and test sets.

This function carves out a test set that contains only entities and relations which also occur in the training set.

Parameters

- **X** (*ndarray, size[n, 3]*) – The dataset to split.
- **test_size** (*int, float*) – If int, the number of triples in the test set. If float, the percentage of total triples.
- **seed** (*int*) – A random seed used to split the dataset.
- **allow_duplication** (*boolean*) – Flag to indicate if the test set can contain duplicated triples.

Returns

- **X_train** (*ndarray, size[n, 3]*) – The training set
- **X_test** (*ndarray, size[n, 3]*) – The test set

Examples

```
>>> import numpy as np
>>> from ampligraph.evaluation import train_test_split_no_unseen
>>> # load your dataset to X
>>> X = np.array([['a', 'y', 'b'],
>>>               ['f', 'y', 'e'],
>>>               ['b', 'y', 'a'],
>>>               ['a', 'y', 'c'],
>>>               ['c', 'y', 'a'],
>>>               ['a', 'y', 'd'],
>>>               ['c', 'y', 'd'],
>>>               ['b', 'y', 'c'],
>>>               ['f', 'y', 'e']])
>>> # if you want to split into train/test datasets
>>> X_train, X_test = train_test_split_no_unseen(X, test_size=2)
>>> X_train
array([['a', 'y', 'b'],
    ['f', 'y', 'e'],
    ['b', 'y', 'a'],
    ['c', 'y', 'a'],
    ['c', 'y', 'd'],
    ['b', 'y', 'c'],
    ['f', 'y', 'e']], dtype='<U1')
>>> X_test
array([['a', 'y', 'c'],
    ['a', 'y', 'd']], dtype='<U1')
>>> # if you want to split into train/valid/test datasets, call it 2 times
>>> X_train_valid, X_test = train_test_split_no_unseen(X, test_size=2)
>>> X_train, X_valid = train_test_split_no_unseen(X_train_valid, test_size=2)
>>> X_train
array([['a', 'y', 'b'],
    ['b', 'y', 'a'],
    ['c', 'y', 'd'],
    ['b', 'y', 'c'],
    ['f', 'y', 'e']], dtype='<U1')
>>> X_valid
array([['f', 'y', 'e'],
    ['c', 'y', 'a']], dtype='<U1')
>>> X_test
array([['a', 'y', 'c'],
    ['a', 'y', 'd']], dtype='<U1')
```

create_mappings

`ampligraph.evaluation.`**`create_mappings`**`(`*X*`)`

Create string-IDs mappings for entities and relations.

Entities and relations are assigned incremental, unique integer IDs. Mappings are preserved in two distinct dictionaries, and counters are separated for entities and relations mappings.

Parameters **X** (*ndarray, shape [n, 3]*) – The triples to extract mappings.

Returns

- **rel_to_idx** (*dict*) – The relation-to-internal-id associations
- **ent_to_idx** (*dict*) – The entity-to-internal-id associations.

to_idx

`ampligraph.evaluation.to_idx(X, ent_to_idx, rel_to_idx)`

Convert statements (triples) into integer IDs.

Parameters

- **X** (*ndarray*) – The statements to be converted.
- **ent_to_idx** (*dict*) – The mappings between entity strings and internal IDs.
- **rel_to_idx** (*dict*) – The mappings between relation strings and internal IDs.

Returns X – The ndarray of converted statements.

Return type ndarray, shape [n, 3]

3.3.4 Utils

This module contains utility functions for neural knowledge graph embedding models.

Saving/Restoring Models

Models can be saved and restored from disk. This is useful to avoid re-training a model.

save_model(model[, model_name_path])	Save a trained model to disk.
restore_model([model_name_path])	Restore a saved model from disk.

save_model

`ampligraph.utils.save_model(model, model_name_path=None)`

Save a trained model to disk.

Examples

```
>>> import numpy as np
>>> from ampligraph.latent_features import ComplEx
>>> from ampligraph.utils import save_model
>>> model = ComplEx(batches_count=2, seed=555, epochs=20, k=10)
>>> X = np.array([['a', 'y', 'b'],
>>>               ['b', 'y', 'a'],
>>>               ['a', 'y', 'c'],
>>>               ['c', 'y', 'a'],
>>>               ['a', 'y', 'd'],
>>>               ['c', 'y', 'd'],
>>>               ['b', 'y', 'c'],
>>>               ['f', 'y', 'e']])
>>> model.fit(X)
>>> y_pred_before = model.predict(np.array([['f', 'y', 'e'], ['b', 'y', 'd']]))
>>> example_name = 'helloworld.pkl'
>>> save_model(model, model_name_path = example_name)
>>> print(y_pred_before)
[-0.29721245, 0.07865551]
```

Parameters

- **model** (EmbeddingModel) – A trained neural knowledge graph embedding model, the model must be an instance of TransE, DistMult, ComplEx, or HolE.
- **model_name_path** (*string*) – The name of the model to be saved. If not specified, a default name model with current datetime is named and saved to the working directory

restore_model

ampligraph.utils.**restore_model**(*model_name_path=None*)

Restore a saved model from disk.

See also *save_model()*.

Examples

```
>>> from ampligraph.utils import restore_model
>>> import numpy as np
>>> example_name = 'helloworld.pkl'
>>> restored_model = restore_model(model_name_path = example_name)
>>> y_pred_after = restored_model.predict(np.array([['f', 'y', 'e'], ['b', 'y', 'd
↪']]))
>>> print(y_pred_after)
[-0.29721245, 0.07865551]
```

Parameters **model_name_path** (*string*) – The name of saved model to be restored. If not specified, the library will try to find the default model in the working directory.

Returns **model** – the neural knowledge graph embedding model restored from disk.

Return type *EmbeddingModel*

Visualization

Functions to visualize embeddings.

create_tensorboard_visualizations(model, loc)	Create Tensorboard visualization files.

create_tensorboard_visualizations

ampligraph.utils.**create_tensorboard_visualizations**(*model*, *loc*, *labels=None*)

Create Tensorboard visualization files.

Note: this will create all the files required by Tensorboard to visualize embeddings, but you must run Tensorboard yourself.

Examples

```
>>> from ampligraph.utils import create_tensorboard_visualizations, restore_model
>>> import numpy as np
>>> example_name = 'helloworld.pkl'
```

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```
>>> restored_model = restore_model(model_name_path = example_name)
>>> output_path = 'model_tensorboard/'
>>> create_tensorboard_visualizations(restored_model, output_path)
```

Parameters

- **model** (EmbeddingModel) – A trained neural knowledge graph embedding model, the model must be an instance of TransE, DistMult, ComplEx, or HolE.
- **loc** (*string*) – Directory where the files are written.
- **labels** (*pd.DataFrame*) – Label(s) for each embedding point in the Tensorboard visualization. Default behaviour is to use the embeddings labels included in the model.

3.4 How to Contribute

3.4.1 Git Repo and Issue Tracking

AmpliGraph repository is available on GitHub.

A list of open issues is available here.

The AmpliGraph Slack channel is available here.

3.4.2 How to Contribute

We welcome community contributions, whether they are new models, tests, or documentation.

You can contribute to AmpliGraph in many ways:

- Raise a bug report
- File a feature request
- Help other users by commenting on the issue tracking system
- Add unit tests
- Improve the documentation
- Add a new graph embedding model (see below)

3.4.3 Adding Your Own Model

The landscape of knowledge graph embeddings evolves rapidly. We welcome new models as a contribution to AmpliGraph, which has been built to provide a shared codebase to guarantee a fair evalaution and comparison acros models.

You can add your own model by raising a pull request.

To get started, read the documentation on how current models have been implemented.

3.4.4 Clone and Install in editable mode

Clone the repository and checkout the `develop` branch. Install from source with pip. use the `-e` flag to enable editable mode:

```
git clone https://github.com/Accenture/AmpliGraph.git
git checkout develop
cd AmpliGraph
pip install -e .
```

3.4.5 Unit Tests

To run all the unit tests:

```
$ pytest tests
```

See pytest documentation for additional arguments.

3.4.6 Documentation

The project documentation is based on Sphinx and can be built on your local working copy as follows:

```
cd docs
make clean autogen html
```

The above generates an HTML version of the documentation under `docs/_built/html`.

3.4.7 Packaging

To build an AmpliGraph custom wheel, do the following:

```
pip wheel --wheel-dir dist --no-deps .
```

3.5 Examples

3.5.1 Train and evaluate an embedding model

```
import numpy as np
from ampligraph.datasets import load_wn18
from ampligraph.latent_features import ComplEx
from ampligraph.evaluation import evaluate_performance, mrr_score, hits_at_n_score

def main():

    # load Wordnet18 dataset:
    X = load_wn18()

    # Initialize a ComplEx neural embedding model with pairwise loss function:
    # The model will be trained for 300 epochs.
    model = ComplEx(batches_count=10, seed=0, epochs=20, k=150, eta=10,
```

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```
                      # Use adam optimizer with learning rate 1e-3
                      optimizer='adam', optimizer_params={'lr':1e-3},
                      # Use pairwise loss with margin 0.5
                      loss='pairwise', loss_params={'margin':0.5},
                      # Use L2 regularizer with regularizer weight 1e-5
                      regularizer='LP', regularizer_params={'p':2, 'lambda':1e-5},
                      # Enable stdout messages (set to false if you don't want to␣
↪display)
                      verbose=True)

    # For evaluation, we can use a filter which would be used to filter out
    # positives statements created by the corruption procedure.
    # Here we define the filter set by concatenating all the positives
    filter = np.concatenate((X['train'], X['valid'], X['test']))

    # Fit the model on training and validation set
    model.fit(X['train'],
              early_stopping = True,
              early_stopping_params = \
                      {
                          'x_valid': X['valid'],       # validation set
                          'criteria':'hits10',         # Uses hits10 criteria for␣
↪early stopping
                          'burn_in': 100,              # early stopping kicks in␣
↪after 100 epochs
                          'check_interval':20,         # validates every 20th epoch
                          'stop_interval':5,           # stops if 5 successive␣
↪validation checks are bad.
                          'x_filter': filter,          # Use filter for filtering out␣
↪positives
                          'corruption_entities':'all', # corrupt using all entities
                          'corrupt_side':'s+o'         # corrupt subject and object␣
↪(but not at once)
                      }
              )



    # Run the evaluation procedure on the test set (with filtering).
    # To disable filtering: filter_triples=None
    # Usually, we corrupt subject and object sides separately and compute ranks
    ranks = evaluate_performance(X['test'],
                                 model=model,
                                 filter_triples=filter,
                                 use_default_protocol=True, # corrupt subj and obj␣
↪separately while evaluating
                                 verbose=True)

    # compute and print metrics:
    mrr = mrr_score(ranks)
    hits_10 = hits_at_n_score(ranks, n=10)
    print("MRR: %f, Hits@10: %f" % (mrr, hits_10))
    # Output: MRR: 0.886406, Hits@10: 0.935000

if __name__ == "__main__":
    main()
```

3.5.2 Model selection

```
from ampligraph.datasets import load_wn18
from ampligraph.latent_features import ComplEx
from ampligraph.evaluation import select_best_model_ranking

def main():

    # load Wordnet18 dataset:
    X_dict = load_wn18()

    model_class = ComplEx

    # Use the template given below for doing grid search.
    param_grid = {
                     "batches_count": [10],
                     "seed": 0,
                     "epochs": [4000],
                     "k": [100, 50],
                     "eta": [5,10],
                     "loss": ["pairwise", "nll", "self_adversarial"],
                     # We take care of mapping the params to corresponding classes
                     "loss_params": {
                         #margin corresponding to both pairwise and adverserial loss
                         "margin": [0.5, 20],
                         #alpha corresponding to adverserial loss
                         "alpha": [0.5]
                     },
                     "embedding_model_params": {
                         # generate corruption using all entities during training
                         "negative_corruption_entities":"all"
                     },
                     "regularizer": [None, "LP"],
                     "regularizer_params": {
                         "p": [2],
                         "lambda": [1e-4, 1e-5]
                     },
                     "optimizer": ["adam"],
                     "optimizer_params":{
                         "lr": [0.01, 0.0001]
                     },
                     "verbose": True
                 }

    # Train the model on all possibile combinations of hyperparameters.
    # Models are validated on the validation set.
    # It returnes a model re-trained on training and validation sets.
    best_model, best_params, best_mrr_train, \
    ranks_test, mrr_test = select_best_model_ranking(model_class, # Class handle of␣
↪the model to be used
                                                       # Dataset
                                                       X_dict,
                                                       # Parameter grid
                                                       param_grid,
                                                       # Use filtered set for eval
                                                       use_filter=True,
                                                       # corrupt subject and objects␣
↪separately during eval
```

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```
                                                            use_default_protocol=True,
                                                            # Log all the model hyperparams␣
↪and evaluation stats
                                                            verbose=True)
    print(type(best_model).__name__, best_params, best_mrr_train, mrr_test)

if __name__ == "__main__":
    main()
```

3.5.3 Get the embeddings

```
import numpy as np
from ampligraph.latent_features import ComplEx

model = ComplEx(batches_count=1, seed=555, epochs=20, k=10)
X = np.array([['a', 'y', 'b'],
              ['b', 'y', 'a'],
              ['a', 'y', 'c'],
              ['c', 'y', 'a'],
              ['a', 'y', 'd'],
              ['c', 'y', 'd'],
              ['b', 'y', 'c'],
              ['f', 'y', 'e']])
model.fit(X)
model.get_embeddings(['f','e'], embedding_type='entity')
```

3.5.4 Save and restore a model

```
import numpy as np
from ampligraph.latent_features import ComplEx
from ampligraph.utils import save_model, restore_model

model = ComplEx(batches_count=2, seed=555, epochs=20, k=10)

X = np.array([['a', 'y', 'b'],
            ['b', 'y', 'a'],
            ['a', 'y', 'c'],
            ['c', 'y', 'a'],
            ['a', 'y', 'd'],
            ['c', 'y', 'd'],
            ['b', 'y', 'c'],
            ['f', 'y', 'e']])

model.fit(X)

#  Use the trained model to predict
y_pred_before = model.predict(np.array([['f', 'y', 'e'], ['b', 'y', 'd']]))
print(y_pred_before)
#[-0.29721245, 0.07865551]

# Save the model
example_name = "helloworld.pkl"
```

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```
save_model(model, model_name_path = example_name)

# Restore the model
restored_model = restore_model(model_name_path = example_name)

# Use the restored model to predict
y_pred_after = restored_model.predict(np.array([['f', 'y', 'e'], ['b', 'y', 'd']]))
print(y_pred_after)
# [-0.29721245, 0.07865551]
```

3.5.5 Split dataset into train/test or train/valid/test

```
import numpy as np
from ampligraph.evaluation import train_test_split_no_unseen
from ampligraph.datasets import load_from_csv

'''
Assume we have a knowledge graph stored in my_folder/my_graph.csv,
and that the content of such file is:

a,y,b
f,y,e
b,y,a
a,y,c
c,y,a
a,y,d
c,y,d
b,y,c
f,y,e
'''

# Load the graph in memory
X = load_from_csv('my_folder', 'my_graph.csv', sep=',')

# To split the graph in train and test sets:
# (In this toy example the test set will include only two triples)
X_train, X_test = train_test_split_no_unseen(X, test_size=2)

print(X_train)

'''
X_train:[['a' 'y' 'b']
         ['f' 'y' 'e']
         ['b' 'y' 'a']
         ['c' 'y' 'a']
         ['c' 'y' 'd']
         ['b' 'y' 'c']
         ['f' 'y' 'e']]
'''

print(X_test)

'''
X_test: [['a' 'y' 'c']
         ['a' 'y' 'd']]
```

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```
'''


# To split the graph in train, validation, and test the method must be called twice:
X_train_valid, X_test = train_test_split_no_unseen(X, test_size=2)
X_train, X_valid = train_test_split_no_unseen(X_train_valid, test_size=2)

print(X_train)
'''
X_train:  [['a' 'y' 'b']
           ['b' 'y' 'a']
           ['c' 'y' 'd']
           ['b' 'y' 'c']
           ['f' 'y' 'e']]
'''

print(X_valid)
'''
X_valid:  [['f' 'y' 'e']
           ['c' 'y' 'a']]
'''

print(X_test)
'''
X_test:  [['a' 'y' 'c']
          ['a' 'y' 'd']]
'''
```

3.6 Performance

3.6.1 Predictive Performance

We report the filtered MR, MRR, Hits@1,3,10 for the most common datasets used in literature.

3.6.2 FB15K-237

Model	MR	MRR	Hits@1	Hits@3	Hits@10	Hyperparameters
TransE	153	0.31	0.22	0.35	0.51	k: 1000; epochs: 4000; eta: 50; loss: self_adversarial; loss_params: alpha: 0.5; margin: 5; optimizer: adam; optimizer_params: lr: 0.0001; embedding_model_params: norm: 1; normalize_ent_emb: false; seed: 0; batches_count: 60
DistMult	568	0.29	0.20	0.32	0.47	k: 400; epochs: 4000; eta: 50; loss: self_adversarial; loss_params: alpha: 1; margin: 1; regularizer: LP; regularizer_params: lambda: 0.0001; p: 2; optimizer: adam; optimizer_params: lr: 0.0005; seed: 0; normalize_ent_emb: false; batches_count: 50
ComplEx	519	0.30	0.20	0.33	0.48	k: 350; epochs: 4000; eta: 30; loss: self_adversarial; loss_params: alpha: 1; margin: 0.5; optimizer: adam; optimizer_params: lr: 0.0001; seed: 0; batches_count: 50
HolE	297	0.28	0.19	0.31	0.46	k: 350; epochs: 4000; eta: 30; loss: self_adversarial; loss_params: alpha: 1 margin: 0.5; optimizer: adam; optimizer_params: lr: 0.0001; seed: 0; batches_count: 50

Note: FB15K-237 validation and test sets include triples with entities that do not occur in the training set. We found 8 unseen entities in the validation set and 29 in the test set. In the experiments we excluded the triples where such entities appear (9 triples in from the validation set and 28 from the test set).

3.6.3 WN18RR

Model	MR	MRR	Hits@1	Hits@3	Hits@10	Hyperparameters
TransE	1536	0.23	0.07	0.35	0.51	k: 200; epochs: 4000; eta: 20; loss: self_adversarial; loss_params: margin: 1; optimizer: adam; optimizer_params: lr: 0.0001; regularizer: LP; regularizer_params: lambda: 1.0e-05; p: 1; seed: 0; normalize_ent_emb: false; embedding_model_params: norm: 1; batches_count: 100;
DistMult	6853	0.44	0.42	0.45	0.50	k: 200; epochs: 4000; eta: 20; loss: self_adversarial; loss_params: margin: 1; optimizer: adam; optimizer_params: lr: 0.0005; seed: 0; normalize_ent_emb: false; batches_count: 25
ComplEx	8214	0.44	0.41	0.45	0.50	k: 200; epochs: 4000; eta: 20; loss: nll; loss_params: margin: 1; optimizer: adam; optimizer_params: lr: 0.0005; seed: 0; batches_count: 10;
HolE	7305	0.47	0.43	0.48	0.53	k: 200; epochs: 4000; eta: 20; loss: self_adversarial; loss_params: margin: 1; optimizer: adam; optimizer_params: lr: 0.0005; seed: 0; batches_count: 50

Note: WN18RR validation and test sets include triples with entities that do not occur in the training set. We found 198 unseen entities in the validation set and 209 in the test set. In the experiments we excluded the triples where such entities appear (210 triples in from the validation set and 210 from the test set).

3.6.4 YAGO3-10

Model	MR	MRR	Hits@1	Hits@3	Hits@10	Hyperparameters
TransE	574	0.24	0.15	0.26	0.41	k: 1000; epochs: 4000; eta: 50; loss: self_adversarial; loss_params: alpha: 0.5; margin: 5; optimizer: adam; optimizer_params: lr: 0.0001; embedding_model_params: norm: 1; normalize_ent_emb: false; seed: 0; batches_count: 150
DistMult	4903	0.49	0.41	0.54	0.63	k: 400; epochs: 4000; eta: 50; loss: self_adversarial; loss_params: alpha: 1; margin: 1; optimizer: adam; optimizer_params: lr: 0.0005; regularizer: LP; regularizer_params: lambda: 0.0001; p: 2; seed: 0; normalize_ent_emb: false; batches_count: 100
ComplEx	7266	0.50	0.42	0.55	0.65	k: 350; epochs: 4000; eta: 30; loss: self_adversarial; loss_params: alpha: 1; margin: 0.5; optimizer: adam; optimizer_params: lr: 0.0001; seed: 0; batches_count: 100
HolE	6201	0.50	0.41	0.55	0.65	k: 350; epochs: 4000; eta: 30; loss: self_adversarial; loss_params: alpha: 1; margin: 0.5; optimizer: adam; optimizer_params: lr: 0.0001; seed: 0; batches_count: 100

Note: YAGO3-10 validation and test sets include triples with entities that do not occur in the training set. We found 22 unseen entities in the validation set and 18 in the test set. In the experiments we excluded the triples where such

entities appear (22 triples in from the validation set and 18 from the test set).

3.6.5 FB15K

Warning: The dataset includes a large number of inverse relations, and its use in experiments has been deprecated. Use FB15k-237 instead.

Model	MR	MRR	Hits@1	Hits@3	Hits@10	Hyperparameters
TransE	105	0.55	0.39	0.68	0.79	k: 150; epochs: 4000; eta: 5; loss: pairwise; loss_params: margin: 0.5; optimizer: adam; optimizer_params: lr: 0.0001; regularizer: LP; regularizer_params: lambda: 0.0001; p: 2; seed: 0; embedding_model_params: norm: 1; normalize_ent_emb: false; batches_count: 10
DistMult	177	0.79	0.74	0.82	0.86	k: 200; epochs: 4000; eta: 20; loss: self_adversarial; loss_params: margin: 1; optimizer: adam; optimizer_params: lr: 0.0005; seed: 0; normalize_ent_emb: false; batches_count: 50
ComplEx	188	0.79	0.76	0.82	0.86	k: 200; epochs: 4000; eta: 20; loss: self_adversarial; loss_params: margin: 1; optimizer: adam; optimizer_params: lr: 0.0005; seed: 0; batches_count: 100
HolE	212	0.80	0.76	0.83	0.87	k: 200; epochs: 4000; eta: 20; loss: self_adversarial; loss_params: margin: 1; optimizer: adam; optimizer_params: lr: 0.0005; seed: 0; batches_count: 50

3.6.6 WN18

Warning: The dataset includes a large number of inverse relations, and its use in experiments has been deprecated. Use WN18RR instead.

Model	MR	MRR	Hits@1	Hits@3	Hits@10	Hyperparameters
TransE	446	0.50	0.18	0.81	0.89	k: 150; epochs: 4000; eta: 5; loss: pairwise; loss_params: margin: 0.5; optimizer: adam; optimizer_params: lr: 0.0001; regularizer: LP; regularizer_params: lambda: 0.0001; p: 2; embedding_model_params: norm: 1; normalize_ent_emb: false; seed: 0; batches_count: 10
DistMult	746	0.83	0.73	0.92	0.95	k: 200; epochs: 4000; eta: 20; loss: nll; loss_params: margin: 1; optimizer: adam; optimizer_params: lr: 0.0005; seed: 0; normalize_ent_emb: false; batches_count: 50
ComplEx	715	0.94	0.94	0.95	0.95	k: 200; epochs: 4000; eta: 20; loss: nll; loss_params: margin: 1; optimizer: adam; optimizer_params: lr: 0.0005; seed: 0; batches_count: 50
HolE	658	0.94	0.93	0.94	0.95	k: 200; epochs: 4000; eta: 20; loss: self_adversarial; loss_params: margin: 1; optimizer: adam; optimizer_params: lr: 0.0005; seed: 0; batches_count: 50

To reproduce the above results:

```
$ cd experiments
$ python predictive_performance.py
```

Note: Running `predictive_performance.py` on all datasets, for all models takes ~43 hours on an Intel Xeon Gold 6142, 64 GB Ubuntu 16.04 box equipped with a Tesla V100 16GB.

Experiments can be limited to specific models-dataset combinations as follows:

```
$ python predictive_performance.py -h
usage: predictive_performance.py [-h] [-d {fb15k,fb15k-237,wn18,wn18rr,yago310}]
                                 [-m {complex,transe,distmult,hole}]

optional arguments:
  -h, --help            show this help message and exit
  -d {fb15k,fb15k-237,wn18,wn18rr,yago310}, --dataset {fb15k,fb15k-237,wn18,wn18rr,
↪yago310}
  -m {complex,transe,distmult,hole}, --model {complex,transe,distmult,hole}
```

3.6.7 Runtime Performance

Training the models on FB15K-237 (`k=200, eta=2, batches_count=100, loss=nll`), on an Intel Xeon Gold 6142, 64 GB Ubuntu 16.04 box equipped with a Tesla V100 16GB gives the following runtime report:

model	seconds/epoch
ComplEx	3.19
TransE	3.26
DistMult	2.61
HolE	3.21

3.7 Bibliography

3.8 Changelog

3.8.1 1.0.2

- Added multiclass loss (#24 and #22)
- Updated the negative generation to speed up evaluation for default protocol.(#74)
- Support for visualization of embeddings using Tensorboard (#16)
- Save models with custom names. (#71)
- Quick fix for the overflow issue for datasets with a million entities. (#61)
- Fixed issues in train_test_split_no_unseen API and updated api (#68)
- Added unit test cases for better coverage of the code(#75)
- Corrupt_sides : can now generate corruptions for training on both sides, or only on subject or object
- Better error messages
- Reduced logging verbosity
- Added YAGO3-10 experiments

- Added MD5 checksum for datasets (#47)
- Addressed issue of ambiguous dataset loaders (#59)
- Renamed 'type' parameter in models.get_embeddings to fix masking built-in function
- Updated String comparison to use equality instead of identity.
- Moved save_model and restore_model to ampligraph.utils (but existing API will remain for several releases).
- Other minor issues (#63, #64, #65, #66)

3.8.2 1.0.1

- evaluation protocol now ranks object and subjects corruptions separately
- Corruption generation can now use entities from current batch only
- FB15k-237, WN18RR loaders filter out unseen triples by default
- Removed some unused arguments
- Improved documentation
- Minor bugfixing

3.8.3 1.0.0

- TransE
- DistMult
- ComplEx
- FB15k, WN18, FB15k-237, WN18RR, YAGO3-10 loaders
- generic loader for csv files
- RDF, ntriples loaders
- Learning to rank evaluation protocol
- Tensorflow-based negatives generation
- save/restore capabilities for models
- pairwise loss
- nll loss
- self-adversarial loss
- absolute margin loss
- Model selection routine
- LCWA corruption strategy for training and eval
- rank, Hits@N, MRR scores functions

3.9 About

AmpliGraph is maintained by Accenture Labs Dublin.

3.9.1 Contact us

The AmpliGraph Slack channel is available here.

You can contact us by email at about@ampligraph.org.

3.9.2 How to Cite

If you like AmpliGraph and you use it in your project, why not starring the project on GitHub!

If you instead use AmpliGraph in an academic publication, cite as:

```
@misc{ampligraph,
 author= {Luca Costabello and
          Sumit Pai and
          Chan Le Van and
          Rory McGrath and
          Nicholas McCarthy},
 title = {{AmpliGraph: a Library for Representation Learning on Knowledge Graphs}},
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 doi   = {10.5281/zenodo.2595043},
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}
```

3.9.3 Contributors

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- Nicholas McCarthy
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3.9.4 License

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