
SEffNet

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Side effect embeddings.

COMMAND LINE INTERFACE

1.1 seffnet

Side Effects Knowledge Graph Embeddings.

```
seffnet [OPTIONS] COMMAND [ARGS]...
```

1.1.1 optimize

Run the optimization pipeline for a given method and graph.

```
seffnet optimize [OPTIONS]
```

Options

- input-path** <input_path>
Input graph file. Only accepted edgelist format.
- training-path** <training_path>
training graph file. Only accepted edgelist format.
- testing-path** <testing_path>
testing graph file. Only accepted edgelist format.
- method** <method>
The NRL method to train the model [required]
Options node2vec|DeepWalk|HOPE|GraRep|LINE|SDNE
- seed** <seed>
- prediction-task** <prediction_task>
The prediction task for the model [required]
Options link_prediction|node_classification
- labels-file** <labels_file>
The labels file for node classification
- trials** <trials>
the number of trials done to optimize hyperparameters
- dimensions-range** <dimensions_range>
the range of dimensions to be optimized

--storage <storage>
SQL connection string for study database. Example: sqlite:///optuna.db

--name <name>
Name for the study

-o, --output <output>
Output study summary

--weighted
True if graph is weighted.

--classifier-type <classifier_type>
Choose type of classifier for predictive model

Options LR|EN|SVM|RF|ENCV

1.1.2 predict

Predict for a given entity.

```
seffnet predict [OPTIONS] CURIE
```

Options

-n, --number-predictions <number_predictions>

-t, --result-type <result_type>

Options chemical|phenotype|target

Arguments

CURIE
Required argument

1.1.3 predictc

Predict for a chemical by SMILES string.

```
seffnet predictc [OPTIONS] SMILES
```

Options

-n, --number-predictions <number_predictions>

-t, --result-type <result_type>

Options chemical|phenotype|target

Arguments

SMILES

Required argument

1.1.4 rebuild

Build all resources from scratch.

```
seffnet rebuild [OPTIONS]
```

1.1.5 repeat

Repeat training n times.

```
seffnet repeat [OPTIONS]
```

Options

--input-path <input_path>

Input graph file. Only accepted edgelist format.

--training-path <training_path>

training graph file. Only accepted edgelist format.

--testing-path <testing_path>

testing graph file. Only accepted edgelist format.

--method <method>

The NRL method to train the model [required]

Options node2vec|DeepWalk|HOPE|GraRep|LINE|SDNE

--evaluation-file <evaluation_file>

The path to save evaluation results.

--dimensions <dimensions>

The dimensions of embeddings.

--number-walks <number_walks>

The number of walks for random-walk methods.

--walk-length <walk_length>

The walk length for random-walk methods.

--window-size <window_size>

The window size for random-walk methods.

--p <p>

The p parameter for node2vec.

--q <q>

The q parameter for node2vec.

--alpha <alpha>

The alpha parameter for SDNE

--beta <beta>
The beta parameter for SDNE

--epochs <epochs>
The epochs for deep learning methods

--kstep <kstep>
The kstep parameter for GraRep

--order <order>
The order parameter for LINE. Could be 1, 2 or 3

--n <n>
number of repeats.

--seed <seed>

--weighted
True if graph is weighted.

--prediction-task <prediction_task>
The prediction task for the model [required]
Options link_prediction|node_classification

--classifier-type <classifier_type>
Choose type of classifier for predictive model
Options LR|EN|SVM|RF|ENCV

--randomization <randomization>
Options xswap|random|node_shuffle

1.1.6 train

Train my model.

```
seffnet train [OPTIONS]
```

Options

--input-path <input_path>
Input graph file. Only accepted edgelist format.

--training-path <training_path>
training graph file. Only accepted edgelist format.

--testing-path <testing_path>
testing graph file. Only accepted edgelist format.

--seed <seed>

--method <method>
The NRL method to train the model [required]
Options node2vec|DeepWalk|HOPE|GraRep|LINE|SDNE

--evaluation
If true, a testing set will be used to evaluate model.

```

--evaluation-file <evaluation_file>
    The path to save evaluation results.

--embeddings-path <embeddings_path>
    The path to save the embeddings file

--predictive-model-path <predictive_model_path>
    The path to save the prediction model

--training-model-path <training_model_path>
    The path to save the model used for training

--dimensions <dimensions>
    The dimensions of embeddings.

--number-walks <number_walks>
    The number of walks for random-walk methods.

--walk-length <walk_length>
    The walk length for random-walk methods.

--window-size <window_size>
    The window size for random-walk methods.

--p <p>
    The p parameter for node2vec.

--q <q>
    The q parameter for node2vec.

--alpha <alpha>
    The alpha parameter for SDNE

--beta <beta>
    The beta parameter for SDNE

--epochs <epochs>
    The epochs for deep learning methods

--kstep <kstep>
    The kstep parameter for GraRep

--order <order>
    The order parameter for LINE. Could be 1, 2 or 3

--classifier-type <classifier_type>
    Choose type of classifier for predictive model

    Options LRIEN|SVM|RF|ENCV

--weighted
    True if graph is weighted.

--prediction-task <prediction_task>
    The prediction task for the model [required]

    Options link_prediction|node_classification

--labels-file <labels_file>
    The labels file for node classification

```

1.1.7 update

Update node2vec training model.

```
seffnet update [OPTIONS]
```

Options

--updated-graph <updated_graph>
an edgelist containing the graph with new nodes

--chemicals-list <chemicals_list>
a file containing list of chemicals to update the model with

--old-graph <old_graph>
The graph needed to be updated. In pickle format

--updated-graph-path <updated_graph_path>
The path to save the updated fullgraph [required]

--chemsim-graph-path <chemsim_graph_path>
The path to save the chemical similarity graph [required]

--training-model-path <training_model_path>
The path to save the model used for training [required]

--new-training-model-path <new_training_model_path>
the path of the updated training model [required]

--embeddings-path <embeddings_path>
The path to save the embeddings file

--predictive-model-path <predictive_model_path>
The path to save the prediction model

--seed <seed>

1.1.8 web

Run the RESTful API.

```
seffnet web [OPTIONS]
```

Options

--host <host>

--port <port>

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C
CURIE

```

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