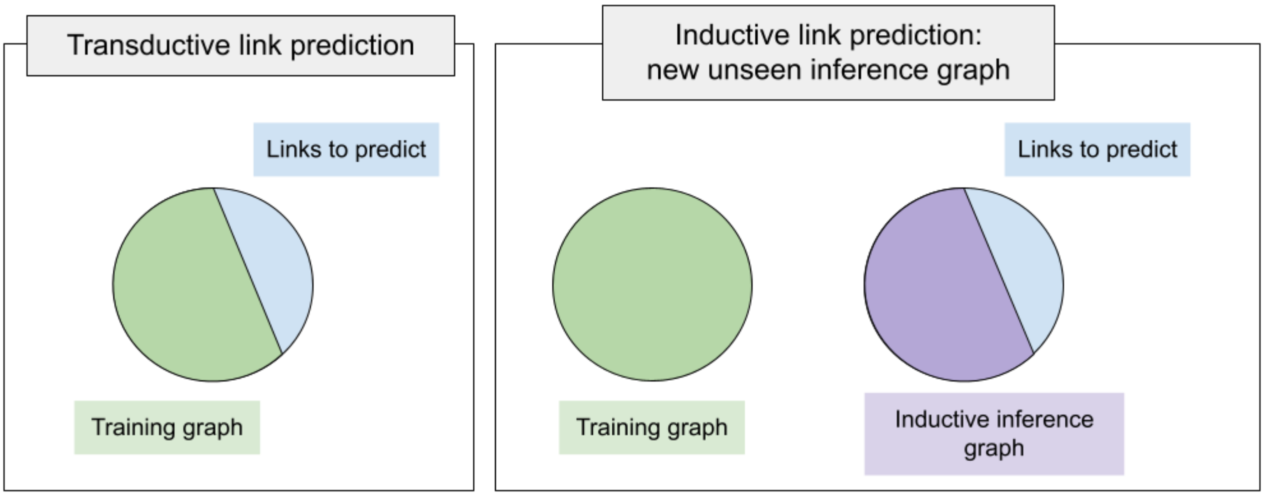
# Inductive Link Prediction




For years, a standard training setup in PyKEEN and other KGE libraries was implying that a training graph includes all entities on which we will run inference (validation, test, or custom predictions). That is, the missing links to be predicted connect already *seen* entities within the train graph. Such a link prediction setup is called **transductive** setup.

What if at inference time we have new, *unseen* entities, and want to predict links between unseen entities? Such setups are unified under the **inductive** framework. Illustrating the difference on the Figure above, the main difference of the inductive setup is that at inference time we have a new graph (called *inductive inference* graph), and link prediction is executed against that new inference graph of unseen entities.

In fact, there exist several variations of the inductive setup according to the taxonomy by [ali2021] :

- An inference graph is totally disconnected from the training graph (disjoint), aka *fully-inductive* setup. Link prediction pattern between entities is therefore *unseen-to-unseen*.
- An inference graph extends the training graph connecting new nodes to the seen graph aka *semi-inductive* setup. Link prediction patterns can be *unseen-to-unseen* when we predict links among newly added nodes or *unseen-to-seen* / *seen-to-unseen* when we predict links between known nodes and newly arrived.

PyKEEN supports inductive link prediction providing interfaces to organize the datasets, build representations of unseen entities, and apply any existing interaction function on top of them. Most importantly, the set of relations **must** be seen at training time. That is, relations seen at inference time must be a subset of training ones because we will learn representations of those relations to transfer to unseen graphs.

# Organizing the Dataset

The basic class to build inductive datasets is `pykeen.datasets.inductive.InductiveDataset`. It is supposed to contain more than 3 triple factories, i.e., in the *fully-inductive* setup it is expected to have at least 4 triple factories (*transductive_training*, *inductive_inference*, *inductive_validation*, *inductive_test*). *transductive_training* is the graph with entities index *(0..N)* on which we will train a model, *inductive_inference* is the new graph appearing at inference time with new entities (indexing *(0..K)*). Note that the number of entities in the *transductive_training* and *inductive_inference* is different. *inductive_validation* and *inductive_test* share the entities with *inductive_inference* but not with *transductive_training*. This way, we inform a model that we are predicting links against the inductive inference graph, not against the training graph.

PyKEEN supports 12 fully-inductive datasets introduced by [teru2020] where training and inductive inference graphs are disjoint. Each of 3 KG families, *InductiveFB15k237*, *InductiveWN18RR*, and *InductiveNELL*, have 4 versions varying by the size of training and inference graphs as well as the total number of entities and relations. It is ensured that the relations sets of all inference graphs are subsets of their training graphs.

# Featurizing Unseen Entities

Training entity embeddings on the training graph is meaningless as those embeddings cannot be used at inference time. Instead, we need some universal featurizing mechanism which would build representations of both seen and unseen entities. In PyKEEN, there exist at least 2 such mechanisms depending on the availability of node descriptions.

## NodePiece

In the most basic case, unseen entities arrive without any features nor descriptions. We cater for this case using `pykeen.nn.representation.NodePieceRepresentation` - since the set of relations at training and inference time is the same, NodePiece Representation will *tokenize* each entity through a subset of incident relation types. Out of computational reasons, NodePiece representations of *inductive_inference* entities (to be seen at inference time) can be pre-computed as well.

At the moment, PyKEEN provides two inductive NodePiece implementations: * `pykeen.models.inductive.InductiveNodePiece` - basic version; * `pykeen.models.inductive.InductiveNodePieceGNN` - in addition to tokenization and learnable hash encoder, this version also performs message passing over the *inductive_inference* graph after building node representations from the vocabulary. By default, message passing is performed with a 2-layer CompGCN

Both inductive versions of NodePiece train an encoder on top of the vocabulary of relational *tokens* that can be easily re-used at inference time. This way, we can obtain representations of unseen entities. *InductiveNodePiece* and *InductiveNodePieceGNN* can be paired with any interaction function from PyKEEN where the dimension of relation vectors is the same as dimension of final node vectors. Alternative interactions can be integrated with custom initialization of the relation representation module.

Let's create a basic *InductiveNodePiece* using one of the *InductiveFB15k237* datasets:

```
from pykeen.datasets.inductive.ilp_teru import InductiveFB15k237
from pykeen.models.inductive import InductiveNodePiece
from pykeen.losses import NSSALoss

dataset = InductiveFB15k237(version="v1", create_inverse_triples=True)

model = InductiveNodePiece(
    triples_factory=dataset.transductive_training,  # training factory, used to tokenize
training nodes
    inference_factory=dataset.inductive_inference,  # inference factory, used to tokenize
inference nodes
    num_tokens=12,  # length of a node hash - how many unique relations per node will be used
    aggregation="mlp",  # aggregation function, defaults to an MLP, can be any PyTorch function
    loss=NSSALoss(margin=15),  # dummy loss
    random_seed=42,
)
```

Creating a message-passing version of NodePiece is pretty much the same:

```
from pykeen.datasets.inductive.ilp_teru import InductiveFB15k237
from pykeen.models.inductive import InductiveNodePieceGNN
from pykeen.losses import NSSALoss

dataset = InductiveFB15k237(version="v1", create_inverse_triples=True)

model = InductiveNodePieceGNN(
    triples_factory=dataset.transductive_training,  # training factory, will be also used for a
GNN
    inference_factory=dataset.inductive_inference,  # inference factory, will be used for a GNN
    num_tokens=12,  # length of a node hash - how many unique relations per node will be used
    aggregation="mlp",  # aggregation function, defaults to an MLP, can be any PyTorch function
    loss=NSSALoss(margin=15),  # dummy loss
    random_seed=42,
    gnn_encoder=None,  # defaults to a 2-layer CompGCN with DistMult composition function
)
```

Note this version has the `gnn_encoder` argument - keeping it `None` would invoke a default 2-layer CompGCN. You can pass here any relational GNN that returns updated matrices of entities and relations as the scoring function will use them for ranking triples. See `pykeen.models.inductive.InductiveNodePieceGNN` for more details.

### Label-based Transformer Representation

If entity descriptions are available, the universal featurizing mechanism can be a language model accessible via `pykeen.nn.representation.LabelBasedTransformerRepresentation`. At both training and inference time, fixed-size entity vectors are obtained after passing their textual descriptions through a pre-trained language model.

This is work in progress and not yet available.

## Training & Evaluation

Generally, training and evaluation of inductive models uses similar interfaces: sLCWA and LCWA training loops, and RankBasedEvaluator. The important addition of inductive interfaces is the *mode* argument. When set to *mode="training"*, an inductive model has to invoke representations of the training graph, when set to *mode=validation* or *mode=testing*, the model has to invoke representations of inference graphs. In the case of fully-inductive (disjoint) datasets from [teru2020] the inference graph at validation and test is the same.

By default, you can use standard PyKEEN training loops `pykeen.training.SLCWATrainingLoop` and `pykeen.training.LCWATrainingLoop` with the new *mode* parameter. Similarly, you can use a standard evaluator `pykeen.evaluation.rank_based_evaluator.RankBasedEvaluator` with the *mode* parameter to evaluate validation / test triples over the whole inference graph.

Moreover, original work of [teru2020] used a restricted evaluation protocol ranking each validation / test triple only against 50 random negatives. PyKEEN implements this protocol with `pykeen.evaluation.rank_based_evaluator.SampledRankBasedEvaluator`

Let's create a training loop and validation / test evaluators:

```
from pykeen.datasets.inductive.ilp_teru import InductiveFB15k237
from pykeen.training import SLCWATrainingLoop
from pykeen.evaluation.rank_based_evaluator import SampledRankBasedEvaluator
from pykeen.losses import NSSALoss

dataset = InductiveFB15k237(version="v1", create_inverse_triples=True)

model = ...  # model init here, one of InductiveNodePiece
optimizer = ...  # some optimizer

training_loop = SLCWATrainingLoop(
    triples_factory=dataset.transductive_training,  # training triples
    model=model,
    optimizer=optimizer,
    mode="training",   # necessary to specify for the inductive mode - training has its own set
of nodes
)

valid_evaluator = SampledRankBasedEvaluator(
    mode="validation",   # necessary to specify for the inductive mode - this will use
inference nodes
    evaluation_factory=dataset.inductive_validation,  # validation triples to predict
    additional_filter_triples=dataset.inductive_inference.mapped_triples,   # filter out true
inference triples
)

test_evaluator = SampledRankBasedEvaluator(
    mode="testing",   # necessary to specify for the inductive mode - this will use inference
nodes
    evaluation_factory=dataset.inductive_testing,  # test triples to predict
    additional_filter_triples=dataset.inductive_inference.mapped_triples,   # filter out true
inference triples
)
```

## Full Inductive LP Example

A minimally working example for training an *InductiveNodePieceGNN* on the *InductiveFB15k237* (v1) in the sLCWA mode with 32 negative samples per positive, with NSSALoss, and SampledEvaluator would look like this:

```
from pykeen.datasets.inductive.ilp_teru import InductiveFB15k237
from pykeen.models.inductive import InductiveNodePieceGNN
from pykeen.training import SLCWATrainingLoop
from pykeen.evaluation.rank_based_evaluator import SampledRankBasedEvaluator
from pykeen.stoppers import EarlyStopper

from torch.optim import Adam

dataset = InductiveFB15k237(version="v1", create_inverse_triples=True)

model = InductiveNodePieceGNN(
    triples_factory=dataset.transductive_training,  # training factory, will be also used for a
GNN
    inference_factory=dataset.inductive_inference,  # inference factory, will be used for a GNN
    num_tokens=12,  # length of a node hash - how many unique relations per node will be used
    aggregation="mlp",  # aggregation function, defaults to an MLP, can be any PyTorch function
    loss=NSSALoss(margin=15),  # dummy loss
    random_seed=42,
    gnn_encoder=None,  # defaults to a 2-layer CompGCN with DistMult composition function
)

optimizer = Adam(params=model.parameters(), lr=0.0005)

training_loop = SLCWATrainingLoop(
    triples_factory=dataset.transductive_training,  # training triples
    model=model,
    optimizer=optimizer,
    negative_sampler_kwargs=dict(num_negs_per_pos=32)
    mode="training",   # necessary to specify for the inductive mode - training has its own set
of nodes
)

# Validation and Test evaluators use a restricted protocol ranking against 50 random negatives
valid_evaluator = SampledRankBasedEvaluator(
    mode="validation",   # necessary to specify for the inductive mode - this will use
inference nodes
    evaluation_factory=dataset.inductive_validation,  # validation triples to predict
    additional_filter_triples=dataset.inductive_inference.mapped_triples,   # filter out true
inference triples
)

# According to the original code
#
https://github.com/kkteru/grail/blob/2a3dffa719518e7e6250e355a2fb37cd932de91e/test_ranking.py#L52
L529
# test filtering uses only the inductive_inference split and does not include
inductive_validation triples
# If you use the full RankBasedEvaluator, both inductive_inference and inductive_validation
triples
# must be added to the additional_filter_triples
test_evaluator = SampledRankBasedEvaluator(
    mode="testing",   # necessary to specify for the inductive mode - this will use inference
nodes
    evaluation_factory=dataset.inductive_testing,  # test triples to predict
    additional_filter_triples=dataset.inductive_inference.mapped_triples,   # filter out true
inference triples
)

early_stopper = EarlyStopper(
    model=model,
    training_triples_factory=dataset.inductive_inference,
    evaluation_triples_factory=dataset.inductive_validation,
    frequency=1,
```

```
    patience=100000,  # for test reasons, turn it off
    result_tracker=None,
    evaluation_batch_size=256,
    evaluator=valid_evaluator,
)

# Training starts here
training_loop.train(
    triples_factory=dataset.transductive_training,
    stopper=early_stopper,
    num_epochs=100,
)

# Test evaluation
result = test_evaluator.evaluate(
    model=model,
    mapped_triples=dataset.inductive_testing.mapped_triples,
    additional_filter_triples=dataset.inductive_inference.mapped_triples,
    batch_size=256,
)

# print final results
print(result.to_flat_dict())
```