

# Knowledge Graph Embeddings for Downstream Machine Learning Tasks with RDF2Vec

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Ir. Bram STEENWINCKEL

IDLab

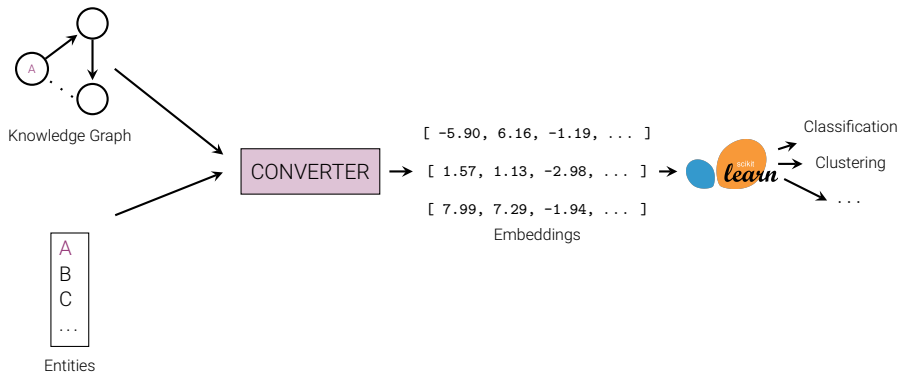
- Influential research group of imec.
- Focuses on Internet technologies and data science.
- Makes contributions to future global standards (e.g., W3C and 5G).
- Located at the University of Ghent and the University of Antwerp.
- Counts more than 500 collaborators.

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<sup>1</sup>Internet Technology & Data Science Lab.

- Associated with the Master's Thesis over a period of 16 weeks.
- Took place within the Knowledge Management team of the IDLab's Discover research center cluster which optimizes intelligent agents and their interactions.
- The Knowledge Management team created more than twenty research projects.

# Motivation



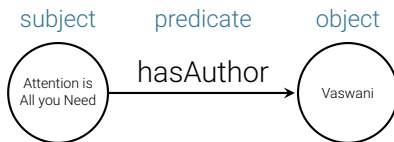


Figure: Triple.

Example of URI<sup>2</sup>:  $\underbrace{\text{http://dl-learner.org/carcinogenesis}}_{\text{URL}^3} \underbrace{\text{\#d187}}_{\text{URN}^4}$

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<sup>2</sup>Uniform Resource Identifier.

<sup>3</sup>Uniform Resource Locator.

<sup>4</sup>Uniform Resource Name.

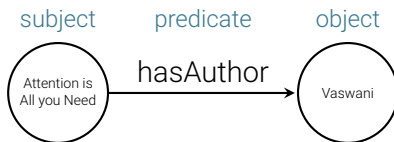


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# Knowledge Graph

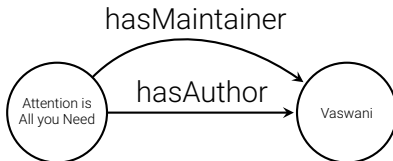


Figure: Knowledge Graph (KG).

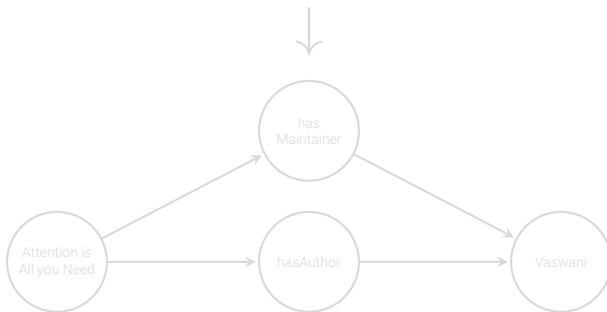


Figure: Oriented Graph.

# Knowledge Graph

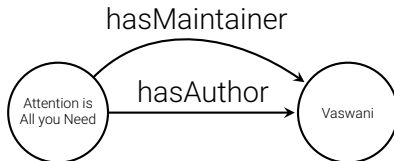


Figure: Knowledge Graph (KG).

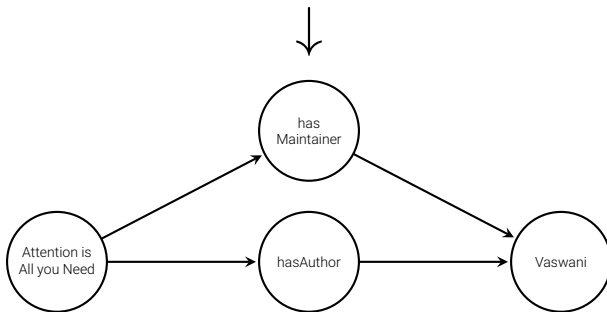
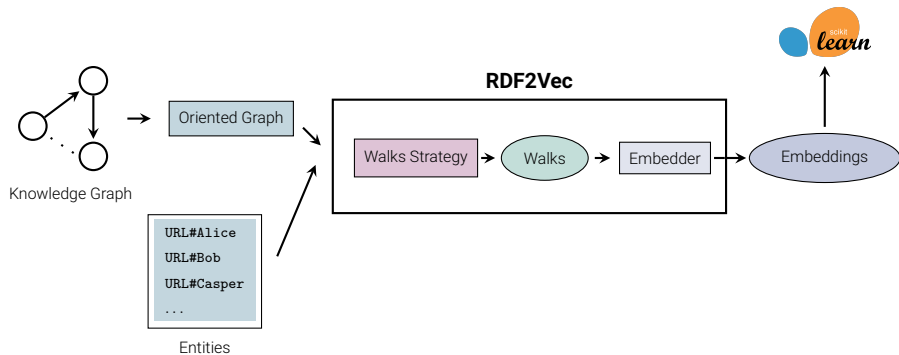


Figure: Oriented Graph.

# RDF2Vec<sup>5</sup>

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<sup>5</sup>Resource Description Framework To Vector.



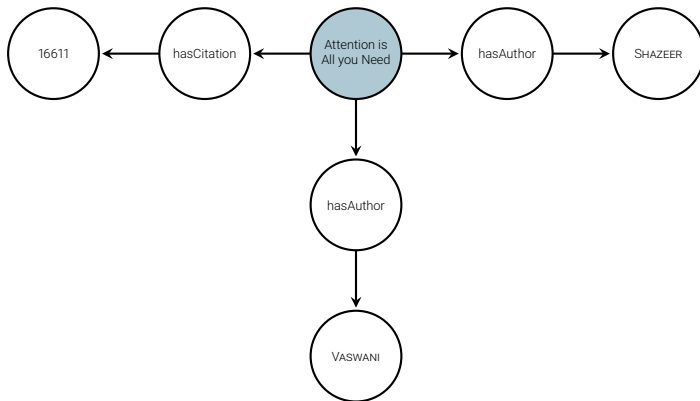


Figure: Walk Extraction for an Oriented Graph (Part I).

Walk Extraction: Attention is All you Need

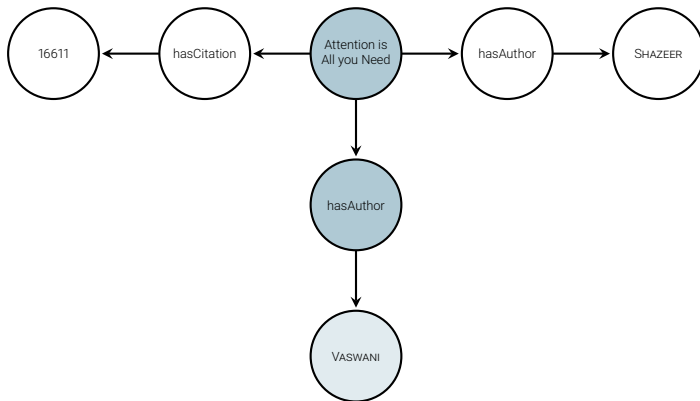


Figure: Walk Extraction for an Oriented Graph (Part II).

Walk Extraction: Attention is All you Need → hasAuthor

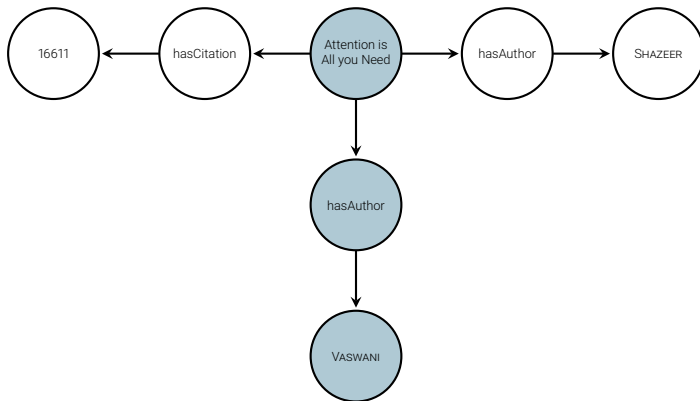


Figure: Walk Extraction for an Oriented Graph (Part III).

Walk Extraction: **Attention is All you Need** → **hasAuthor** → **VASWANI**

# Internship



# Scope of the Internship

Consists in improving `pyRDF2Vec`:

- ➊ Add better support for different KG sizes.
- ➋ Add first support of *literals*.
- ➌ Avoid re-training a model when new nodes<sup>6</sup> are added in the KG.
- ➍ Improve the documentation of the library.
- ➎ Add Continuous Integration / Delivery / Testing.

Where the goals are *ordered according to importance*.

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<sup>6</sup>Also called *vertices*.

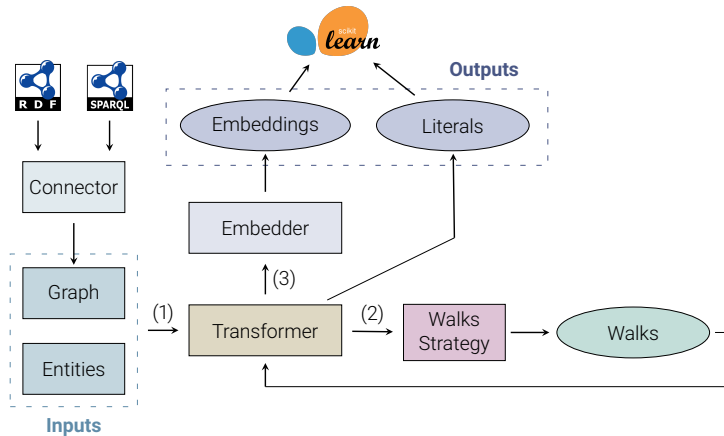


Figure: Workflow of pyRDF2Vec.

Consists of reducing the walk extraction time by using:

- a cache memory;
- multiprocessing;
- cache pre-filling;
- an appropriate data structure for the nodes;
- a connection pool;
- ...

# Optimization Mechanism Results

<b>Data Set</b>	<b>Triples</b>	<b>Entities</b>	<b>Relations</b>	<b>Size</b>
MUTAG	74,567	22,534	24	small
AM	5,700,371	933,471	100	medium
DBP:Cities	651,580,976	4,233,000	7,992	large

**Table:** Properties of the Data Sets Used for the Benchmarks.

Performed on the IDLab's servers with **4 CPUs** and **64 GB** RAM.

Data Set	Speedup		
	Minimum	Maximum	Average
MUTAG	6.20	13.28	9.74
AM	1.44	8.94	5.19
DBP:Cities	2.22	3.23	2.72

Table: Speedup Results with Optimization Mechanisms.

- caching and pre-filling benefit small KGs like MUTAG the most;
- multiprocessing is more interesting for large KGs like DBP:Cities.

# Literals

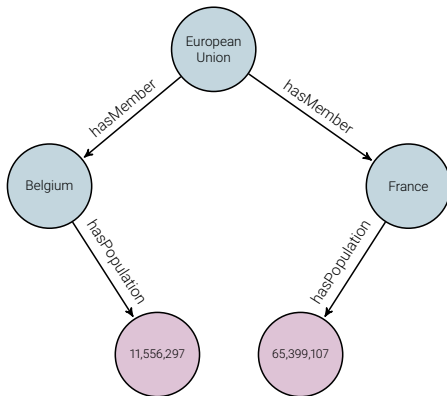


Figure: Oriented Graph with 5 Nodes and 4 Edges.



# Literals

Literals may:

- be **specific** to some entities;
- be **too expensive** to extract;
- **not** be **interesting**.

→ Let the user **specify the literals to extract**

For example: [

```
      predicate 1      predicate 2
[ {hasCapital} → {hasLatitude} ], # 50.85; 48.85
[ {hasCapital} → {hasLongitude} ], # 4.35; 2.34
[ {hasPopulation} ], # 11,55; 65,39
...
]
```

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]
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# Online Learning

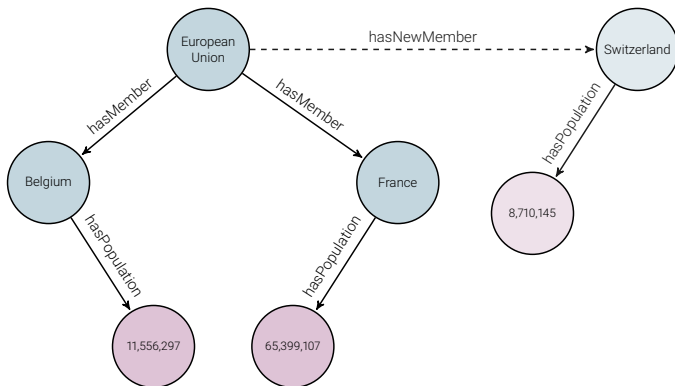


Figure: Oriented Graph With 7 Nodes and 6 Edges.

→ Consists in updating the vocabulary of walks of an initial model.

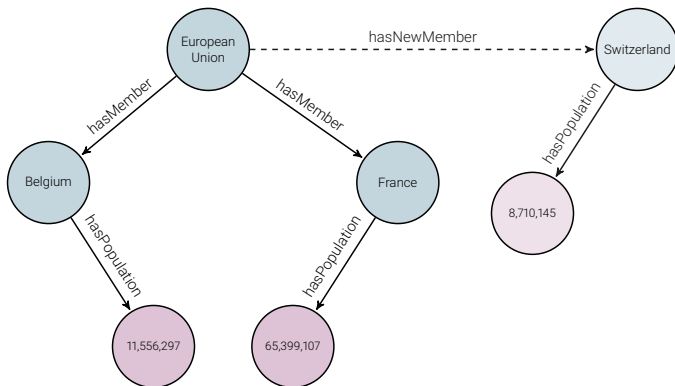


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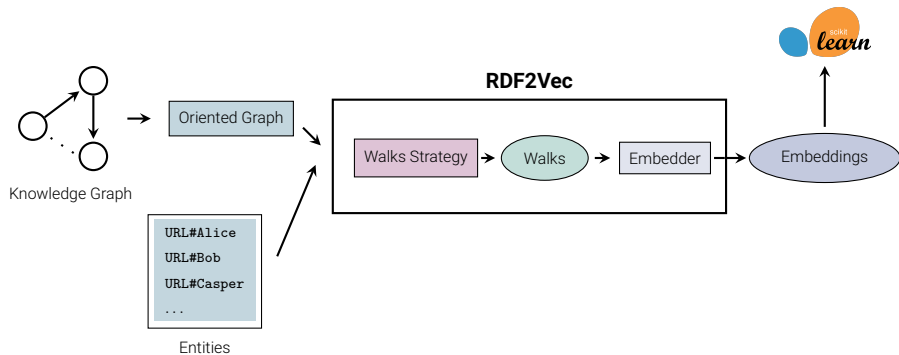
Demo Time! 

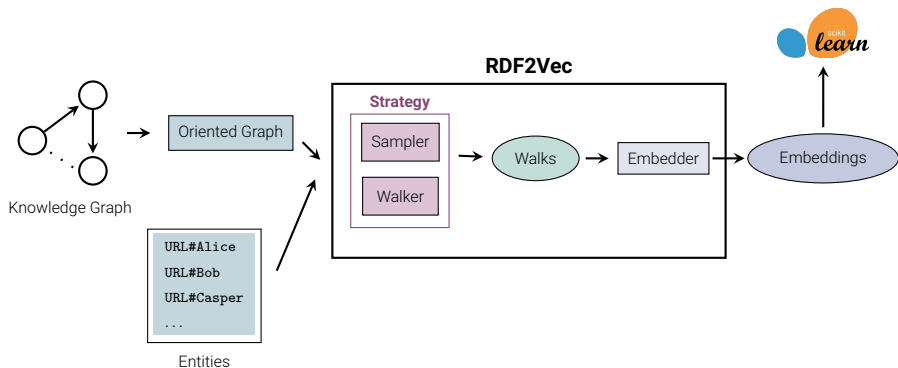
On the menu:

- The `pyRDF2Vec` GitHub repository.
- An example of using literals.
- An example of using ~~online learning~~ (available on GitHub).

## A Trip to Sesame Street: Evaluation of BERT and Other Recent Embedding Techniques Within RDF2Vec







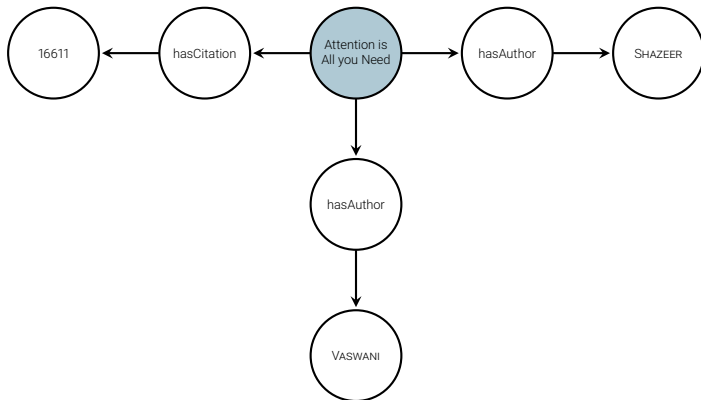


Figure: Oriented Graph.

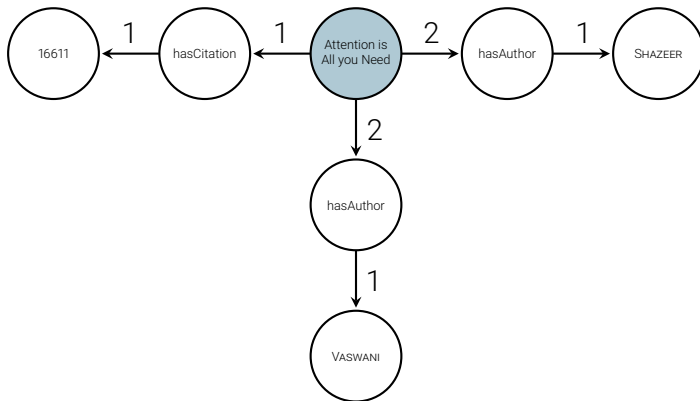


Figure: Walk Extraction for an Oriented Graph (Part I).

Walk Extraction: Attention is All you Need

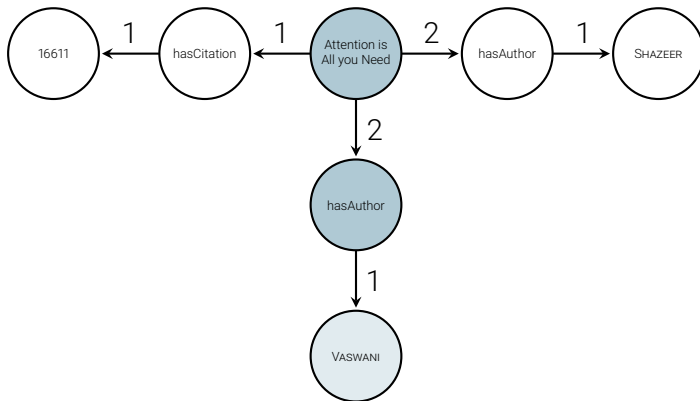


Figure: Walk Extraction for an Oriented Graph (Part II).

Walk Extraction: [Attention is All you Need](#) → [hasAuthor](#)

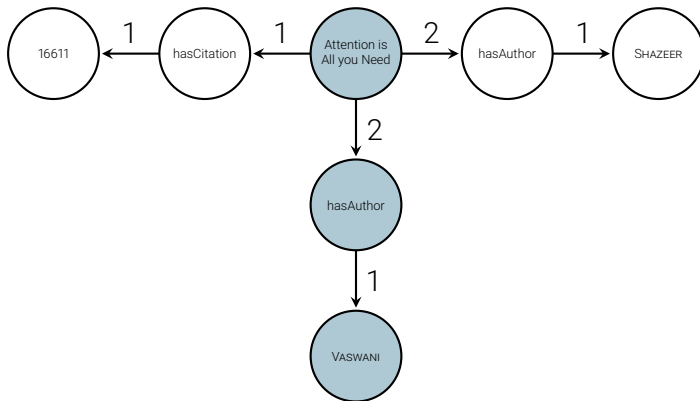
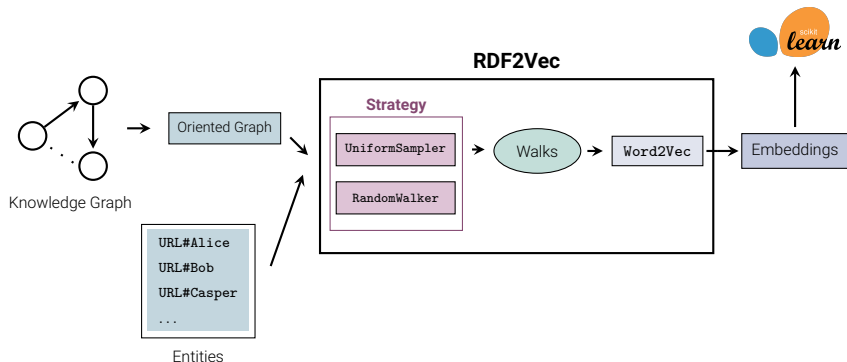
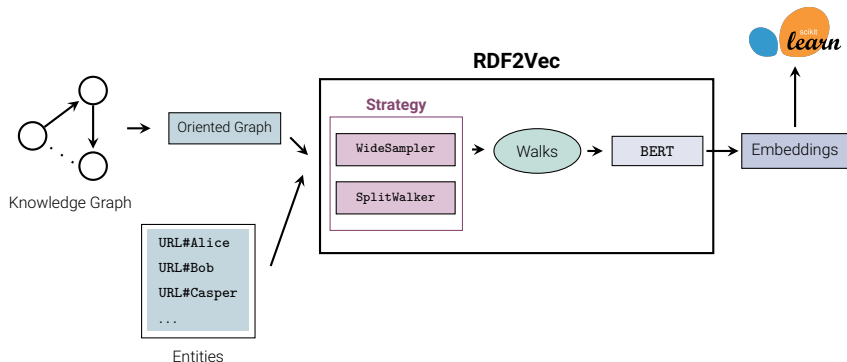


Figure: Walk Extraction for an Oriented Graph (Part III).

Walk Extraction: Attention is All you Need  $\rightarrow$  hasAuthor  $\rightarrow$  VASWANI







# Scope of the Master's Thesis

Mainly consists in evaluating BERT<sup>7</sup> with Word2Vec and implementing other strategies:

- ① Supported BERT and FastText for comparison purposes.
- ② Evaluated the impact of BERT with Word2Vec and FastText.
- ③ SplitWalker as a new walking strategy in RDF2Vec.
- ④ WideSampler as a new sampling strategy in RDF2Vec.

BONUS: has unintentionally improved Word2Vec and pyRDF2Vec.

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<sup>7</sup>Only the traditional BERT model is concerned by this scope.

BERT

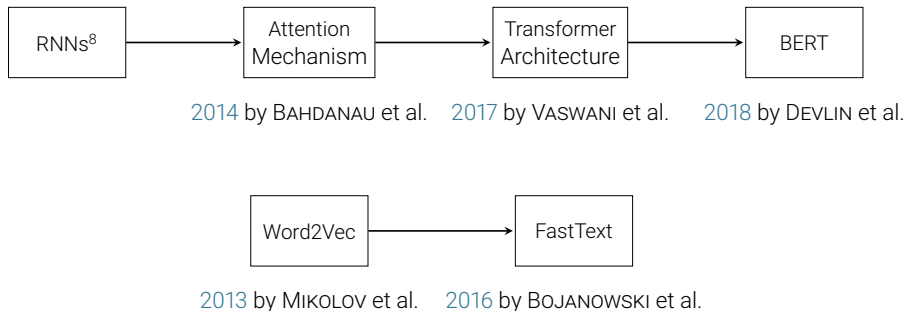


Figure: Summary Timeline.

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<sup>8</sup>Recurrent Neural Networks.

Main characteristics:

- Allows **one or two** input sentences.
- Uses a **WordPiece** tokenization.

**Table:** Example of Tokenization With BERT.

	The	machine	loves	embeddings.					
[CLS]	the	machine	loves	em	##bed	##ding	##s	.	[SEP]
101	1996	3698	7459	7861	8270	4667	2015	1012	102

- Uses **two pre-training phases**:
  - 1 Masked Language Model (MLM);
  - 2 Next Sentence Prediction (NSP).
- Contextualizes embeddings **using bidirectional representations**.

- Build the vocabulary.
- Fit the BERT model in two ways:
  - ① node tokenization: ensuring not to split the nodes;
  - ② training: only done with MLM using a data collator.
- Get entity embeddings.

# Improve the Model's Accuracy of Word2Vec

# Improve the Model's Accuracy of Word2Vec

Table: Context Words Determination for a Window Size of 2.

Input Text	Target Word	Context Words
I will always remember her	i	will always
I will always remember her	will	i always remember
I will always remember her	always	i will remember her
I will always remember her	remember	will always her
I will always remember her	her	always remember

# Improve the Model's Accuracy of Word2Vec

In two ways:

- 1 Extract the parent nodes of an entity.
- 2 Better positioning the entity in the walks to maximize its occurrence in the training samples.

For example:

```
("URL#Alice", "URL#knows", "URL#Bob"),  
("URL#Alice", "URL#loves", "URL#Bob"),  
...
```

May become:

```
("URL#Casper", "URL#raised", "URL#Alice", "URL#knows", "URL#Bob"),  
("URL#Mathilde", "URL#raised", "URL#Alice", "URL#loves", "URL#Bob"),  
...
```



```

1 !cd pyRDF2Vec && PYTHONHASHSEED=10 python examples/word2vec.py

2021-03-21 20:17:54.938323: I tensorflow/stream_executor/platform/default/dso_loader.cc:49] Successfully ope
http://data.bgs.ac.uk/id/EarthMaterialClass/RockName/*~PYSD does not look like a valid URI, trying to serial
http://data.bgs.ac.uk/id/EarthMaterialClass/RockName/*~PYSD does not look like a valid URI, trying to serial
http://data.bgs.ac.uk/id/EarthMaterialClass/RockName/*~PRS does not look like a valid URI, trying to serial
http://data.bgs.ac.uk/id/EarthMaterialClass/RockName/*~PRS does not look like a valid URI, trying to serial
http://data.bgs.ac.uk/id/EarthMaterialClass/RockName/*~PRS does not look like a valid URI, trying to serial
http://data.bgs.ac.uk/id/EarthMaterialClass/RockName/*~SSR does not look like a valid URI, trying to serial
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http://data.bgs.ac.uk/id/EarthMaterialClass/RockName/*~VIS does not look like a valid URI, trying to serial
http://data.bgs.ac.uk/id/EarthMaterialClass/RockName/*~PYSD does not look like a valid URI, trying to serial
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http://data.bgs.ac.uk/id/EarthMaterialClass/RockName/*~SSD does not look like a valid URI, trying to serial
100% 146/146 [00:00<00:00, 346.01it/s]
Extracted 35261 walks for 146 entities (0.5910s)
Fitted 35261 walks (1.9600s)
Predicted 29 entities with an accuracy of 65.5172%
Confusion Matrix ([TN, FP], [FN, TP]):
[[19 0]
 [10 0]]

4 from pyrdf2vec.embedders import Word2Vec
5 from pyrdf2vec.graphs import KG
6 from pyrdf2vec.walkers import RandomWalker
7 from sklearn.manifold import TSNE
8 from sklearn.metrics import accuracy_score, confusion_matrix
9 from sklearn.model_selection import GridSearchCV
10 from sklearn.svm import SVC
11 from transformers import TrainingArguments
12
13 Ensure the determinism of this script by initializing a pseudo-r
14 RANDOM_STATE = 10
15
16 tst_data = pd.read_csv("/content/drive/MyDrive/BGS/BGS_test.tsv",
17 rain_data = pd.read_csv("/content/drive/MyDrive/BGS/BGS_train.tsv
18
19 rain_entities = [entity for entity in train_data["rock"]]
20 rain_labels = list(train_data["label_lithogenesis"])
21
22 tst_entities = [entity for entity in test_data["rock"]]
23 tst_labels = list(test_data["label_lithogenesis"])
24
25 vitites = train_entities + test_entities
26 abels = train_labels + test_labels
27
28 nbddings, _ = RDF2VecTransformer(
29     # Ensure random determinism for Word2Vec
30     # Must be used with PYTHONHASHSEED.
31     Word2Vec(workers=1, iter=1),
32     # Extract all walks with a maximum depth of 2 for each entity.
33     # processes and use a random state to ensure that the same wal
34     # generated for the entities.
35     walkers=[RandomWalker(2, None, n_jobs=2, with reverse=False, r
36     verbose=1,
37     fit transform(
38     KG("/content/drive/MyDrive/BGS/BGS.nt", fmt="nt"),
39     entities,
40
41

```

Figure: Word2Vec (Before Improvement).

```

1 !cd pyRDF2Vec && PYTHONHASHSEED=10 python examples/word2vec.py
2021-03-21 19:41:29.235699: I tensorflow/stream_executor/platform/default/dso_loader.cc:49] Successfully opened dynamic library libcudart.so.10.1
http://data.bgs.ac.uk/id/EarthMaterialClass/RockName/*~PYSD does not look like a valid URI, try
http://data.bgs.ac.uk/id/EarthMaterialClass/RockName/*~PYSD does not look like a valid URI, try
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http://data.bgs.ac.uk/id/EarthMaterialClass/RockName/*~RSR does not look like a valid URI, try
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100% 146/146 [00:07<00:00, 18.60it/s]
Extracted 636620 walks for 146 entities (8.2464s)
Fitted 636620 walks (27.6553s)
Predicted 29 entities with an accuracy of 93.1034%
Confusion Matrix ([[TN, FP], [FN, TP]]):
[[18 1]
 [ 1 9]]

11 from transformers import TrainingArguments
12
13 # Ensure the determinism of this script by initializing a pseudo-random number
14 RANDOM_STATE = 10
15
16 test_data = pd.read_csv("/content/drive/MyDrive/BGS/BGS_test.tsv", sep="\t")
17 train_data = pd.read_csv("/content/drive/MyDrive/BGS/BGS_train.tsv", sep="\t")
18
19 train_entities = [entity for entity in train_data["rock"]]
20 train_labels = list(train_data["label_lithogenesis"])
21
22 test_entities = [entity for entity in test_data["rock"]]
23 test_labels = list(test_data["label_lithogenesis"])
24
25 entities = train_entities + test_entities
26 labels = train_labels + test_labels
27
28 embeddings_ = RDF2VecTransformer(
29     # Ensure random determinism for Word2Vec
30     # Must be used with PYTHONHASHSEED.
31     Word2Vec(workers=1, iter=1),
32     # Extract all walks with a maximum depth of 2 for each entity using two
33     # processes and use a random state to ensure that the same walks are
34     # generated for the entities.
35     walkers=[RandomWalker(2, None, n_jobs=2, with_reverse=True, random_state=
36     verbose=1,
37 ).fit_transform(
38     KG("/content/drive/MyDrive/BGS/BGS.nt", fmt="nt"),
39     entities,
40 )
41
42 train_embeddings = embeddings[: len(train_entities)]
43 test_embeddings = embeddings[len(train_entities):]
44
45 # Fit a Support Vector Machine on train embeddings and pick the best
46 # C-parameters (regularization strength).
47 clf = GridSearchCV(
48     SVC(random_state=RANDOM_STATE), {'C': [10 ** i for i in range(-3, 4)]})

```

Figure: Word2Vec (After Improvement).

# FastText

Table: Sub-word Generation for Character  $N$ -Grams of Length 3, 4, 5, and 6.

Word	Length	Character $n$ -grams
flying	3	<fl, fly, lyi, yin, ing, ng>
	4	<fly, flyi, lyin, ying, ing>
	5	<flyi, lying, ying>
	6	<flyin, flying, lying>

Mainly solves the embeddings creation for Out-Of-Vocabulary words.

Use the `gensim` library by:

- ➊ Removing the `min_n` and `max_n` parameters for *n*-grams splitting.
- ➋ Allowing to compute *n*-grams for walks only<sup>10</sup> by separating the objects and predicates URIs with a splitting function.
- ➌ Avoiding dependency on Cython.

---

<sup>10</sup>The object nodes in `pyRDF2Vec` are encoded in MD5 to reduce their storage in RAM.

<sup>11</sup><https://github.com/IBCNServices/pyRDF2Vec/blob/feature/bert/pyrdf2vec/embedders/fasttext.py>

# Benchmarks

- Varied the maximum:
  - 1 number of walks per entity;
  - 2 depth per walk.
- Performed on **MUTAG**.
- Use 320 training entities and attempt to predict 68 test entities.
- Take the mean and standard deviation of five tests.

Embedding techniques and walking strategies:

- IDLab's servers with 4 CPUs, 64 GB RAM, and one GPU.

Sampling strategies:

- ThinkPad machine with 4 CPUs, 16 GB RAM.

# Benchmarks for Embedding Techniques

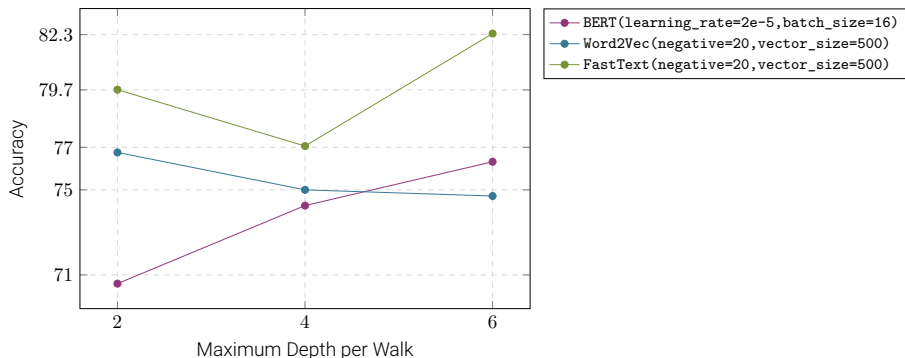


Figure: Embedding Techniques for MUTAG (Maximum Depth per Walk).



# Benchmarks for Embedding Techniques

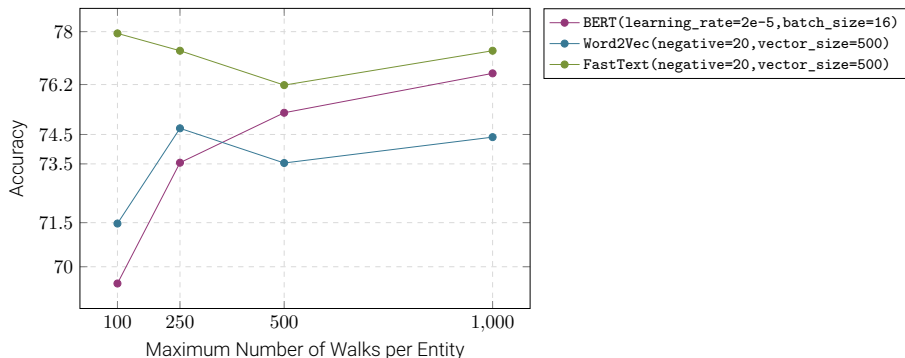


Figure: Embedding Techniques for MUTAG (Maximum Number of Walks).

# Strategies

- Extension of the RandomWalker.
- Based on the principle of preprocessing.
- Customizable by a splitting function.
- Inspired by the way FastText works.

---

<sup>12</sup> <https://github.com/IBCNServices/pyRDF2Vec/blob/master/pyrdf2vec/walkers/split.py>

	Initial Node	Node After Splitting
Walk 1	<a href="http://dl-learner.org/carcinogenesis#d19">http://dl-learner.org/carcinogenesis#d19</a>	<a href="http://dl-learner.org/carcinogenesis#d19">http://dl-learner.org/carcinogenesis#d19</a>
	<a href="http://dl-learner.org/carcinogenesis#hasBond">http://dl-learner.org/carcinogenesis#hasBond</a>	has
	<a href="http://dl-learner.org/carcinogenesis#bond3209">http://dl-learner.org/carcinogenesis#bond3209</a>	bond 3209
Walk 2	<a href="http://dl-learner.org/carcinogenesis#d36">http://dl-learner.org/carcinogenesis#d36</a>	<a href="http://dl-learner.org/carcinogenesis#d36">http://dl-learner.org/carcinogenesis#d36</a>
	<a href="http://www.w3.org/1999/02/22-rdf-syntax-ns#type">http://www.w3.org/1999/02/22-rdf-syntax-ns#type</a>	type
	<a href="http://dl-learner.org/carcinogenesis#bond">http://dl-learner.org/carcinogenesis#bond</a>	bond

Table: Walk Transformation With SplitWalker.

Walker	Average Rank
HALKWalker(freq_threshold=0.01)	1
SplitWalker	2
RandomWalker	3
NGramWalker(grams=3)	4
WalkletWalker	5
AnonymousWalker	6

Table: Average Rank of the Walking Strategies.

- Maximizes the extraction of shared features between entities.
- Assumes that single entity-specific features have a negligible impact on the quality of the generated embeddings.
- Assigns higher weights to edges that lead to the largest number of:
  - 1 predicates and objects in the neighborhood;
  - 2 occurrence of predicates and objects in a graph.

---

<sup>13</sup> <https://github.com/IBCNServices/pyRDF2Vec/blob/master/pyrdf2vec/samplers/wide.py>

Sampler	Average Rank
WideSampler	1
ObjPredFreqSampler(inverse=True)	2
PredFreqSampler	3
ObjFreqSampler	4
ObjFreqSampler(inverse=True)	5
PageRankSampler(inverse=True,alpha=0.85)	6
PageRankSampler(inverse=True,split=True,alpha=0.85)	7
ObjFreqSampler(inverse=True,split=True)	8
PageRankSampler(split=True,alpha=0.85)	9
PredFreqSampler(inverse=True)	10
ObjPredFreqSampler	11
UniformSampler	11
PageRankSampler(alpha=0.85)	12

Table: Average Rank of the Sampling Strategies.

# Future Work



- Inject (subject, object) pairs to BERT instead of pairs of walks.
- Evaluate:
  - the KG-oriented BERT models with other embedding techniques;
  - BERT, SplitWalker and WideSampler on larger KGs.
- If necessary, implement a new KG-oriented BERT model.

# Conclusion

- The traditional BERT model has not been as effective as expected: small gain for the model's accuracy in counterpart of a more important training time and storage space.
- WideSampler and SplitWalker finished first and second respectively in average rank of the MUTAG benchmarks.
- Improved the accuracy of the Word2Vec model.
- Gain in popularity for pyRDF2Vec.

Question Time 

# Appendices

Three categories of conversion algorithms based:

- 1 Direct encoding (e.g., TransE<sup>14</sup>);

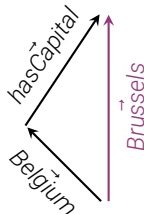


Figure: Embedding Computations With TransE.

- 2 Deep Learning (e.g., R-GCNs<sup>15</sup>);
- 3 Path/Walk (e.g., RDF2Vec<sup>16</sup>).

---

<sup>14</sup>Translating Embeddings.

<sup>15</sup>Modeling Relational Data with Graph Convolutional Networks.

<sup>16</sup>Resource Description Framework To Vector.

# Continuous Bag-of-Words Model

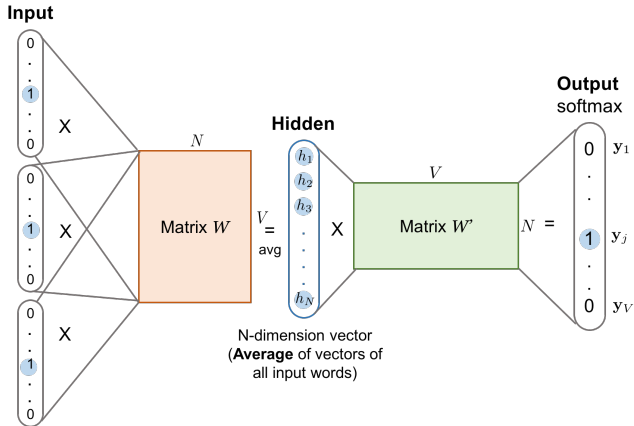


Figure: CBOW Model Architecture.

# Skip-Gram Model

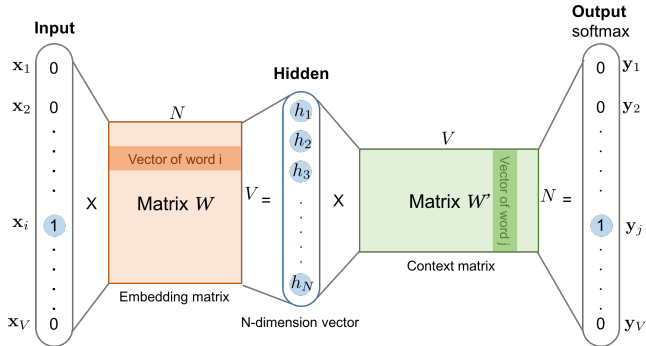


Figure: Skip-Gram Model Architecture.



# Recurrent Neural Networks

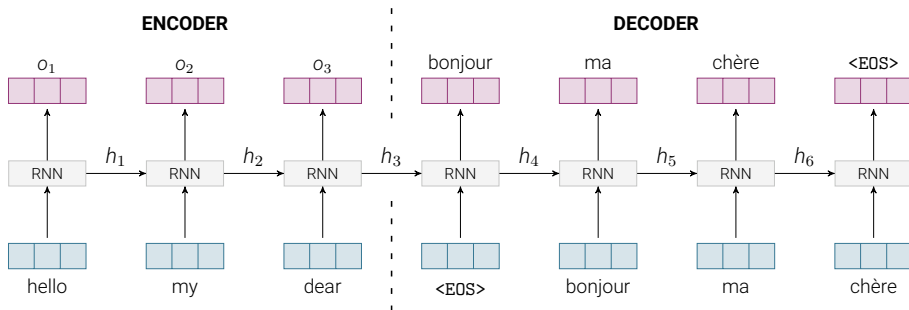


Figure: Sequence-to-Sequence Learning With RNNs.

# Attention Mechanism

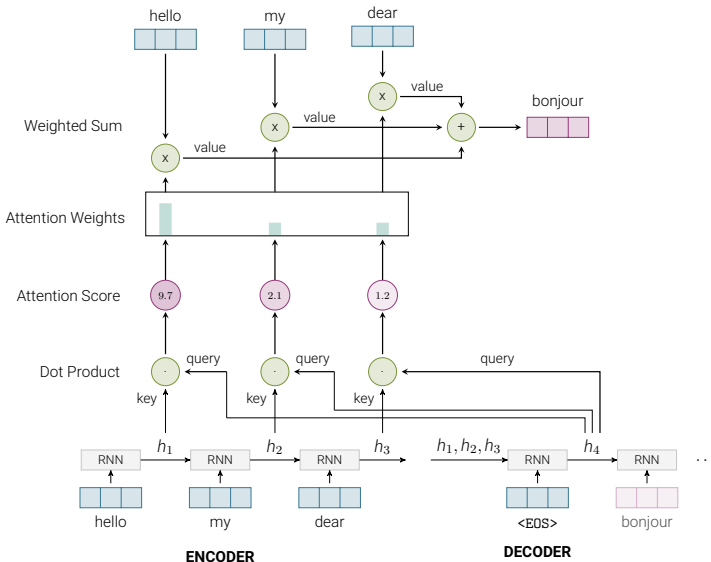


Figure: Seq2Seq Learning With Attention Mechanism.

# Transformer

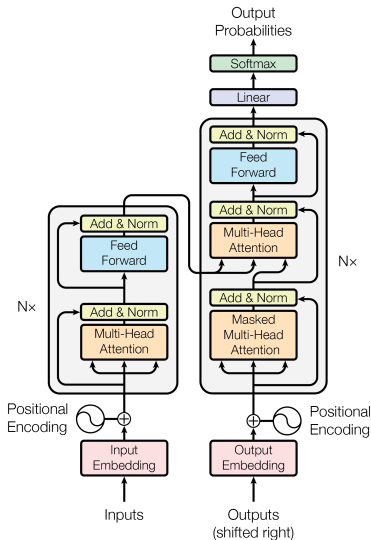


Figure: Transformer Model Architecture.

Source: VASWANI et al. – Attention Is All You Need

# Input Embeddings

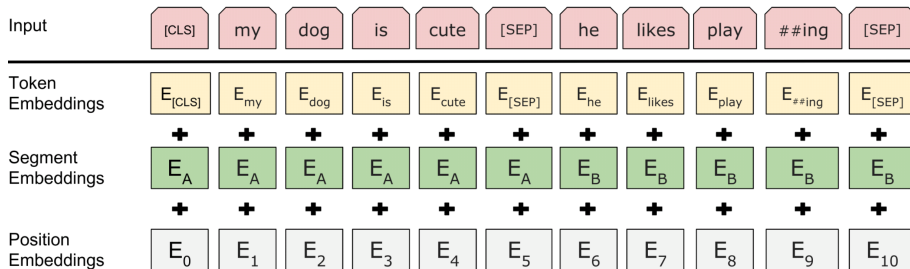


Figure: Example of Sentence Pair Encoding.

Source: DEVLIN et al. – BERT

GNU Emacs is the **best** text editor

- a token is replaced by a [MASK] token in 80 % of the cases;
- a token is replaced randomly in 10 % of the cases;
- a token remains unchanged in 10 % of the cases.

Table: Example of NSP With BERT.

Sentence A	Sentence B	Label
GNU Emacs is the best text editor.	I should use it.	isNextSentence
GNU Emacs is the best text editor.	I have a cat.	NotNextSentence

3: **end if**

### Listing: Splits Nodes of Random Walks with SplitWalker (Part I).

---

```
def basic_split(self, walks):
    canonical_walks = set()
    for walk in walks:
        canonical_walk = [walk[0].name]
        for i, _ in enumerate(walk[1::], 1):
            vertices = []
            if "http" in walk[i].name:
                vertices = " ".join(re.split("[\#]", walk[i].name)).split()
            if i % 2 == 1:
                name = vertices[1] if vertices else walk[i].name
                preds = [
                    sub_name
                    for sub_name in re.split(r"([A-Z][a-z]*)", name)
                    if sub_name
                ]
                for pred in preds:
                    canonical_walk += [pred.lower()]
```



## Listing: Splits Nodes of Random Walks with SplitWalker (Part II).

```
...
else:
    name = vertices[-1] if vertices else walk[i].name
    objs = []
    try:
        objs = [str(float(name))]
    except ValueError:
        objs = re.sub("[^A-Za-z0-9]+", " ", name).split()
        if len(objs) == 1:
            match = re.match(
                r"([a-z]+)([0-9]+)", objs[0], re.I
            )
            if match:
                objs = list(match.groups())
        for obj in objs:
            canonical_walk += [obj.lower()]
        canonical_walk = list(dict(zip(canonical_walk, canonical_walk)))
        canonical_walks.add(tuple(canonical_walk))
    return canonical_walks
```