End-to-End Entity Classification on Multimodal Knowledge Graphs

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Abstract

End-to-end multimodal learning on knowledge graphs has been left largely unaddressed. Instead, most end-to-end models such as message passing networks learn solely from the relational information encoded in graphs’ structure: raw values, or literals, are either omitted completely or are stripped from their values and treated as regular nodes. In either case we lose potentially relevant information which could have otherwise been exploited by our learning methods. To avoid this, we must treat literals and non-literals as separate cases. We must also address each modality separately and accordingly: numbers, texts, images, geometries, et cetera. We propose a multimodal message passing network which not only learns end-to-end from the structure of graphs, but also from their possibly divers set of multimodal node features. Our model uses dedicated (neural) encoders to naturally learn embeddings for node features belonging to five different types of modalities, including images and geometries, which are projected into a joint representation space together with their relational information. We demonstrate our model on a node classification task, and evaluate the effect that each modality has on the overall performance. Our result supports our hypothesis that including information from multiple modalities can help our models obtain a better overall performance.

1 Introduction

The recent adoption of knowledge graphs by multinationals such as Google and Facebook has made them interesting targets for various machine learning applications such as link prediction and node classification. Already, this interest has lead to the development of message passing models which enable data scientists to learn end-to-end from any arbitrary graph. To do so, these models exploit the relational information encoded in the graphs’ structure to guide the learning process. The same approach has also been shown to work quite well on knowledge graphs, obtaining results that are comparable to dedicated models such as RDF2Vec [10] and Weisfeiler-Lehman kernels [12]. Nevertheless, by focusing on a single modality—the graphs’ structure—we are effectively throwing away a lot of other information that knowledge graphs tend to have, and which, if we were able to include them in the learning process, have the potential of

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improving the overall performance of our models.

Combining information from multiple modalities is a topic that is already well studied for information stored in relational form (for instance in relational database management systems). Here too, we often encounter heterogeneous knowledge, containing information from a wide variety of modalities (such as language, audio, or images). In [15], the case is made that to truly learn end-to-end from a collection of heterogeneous, multimodal data, we must design machine learning models that can consume these data in as raw a form as possible, staying as close as we can to the original knowledge, and that we need to adopt a data model which can represent our data in a suitable format, for which the knowledge graph is a natural choice. In other words, even when our heterogeneous multimodal data is not initially represented as a knowledge graph, transforming it to this format is a natural first step in an end-to-end multimodal machine learning pipeline.

In this paper, we aim to show a first proof-of-concept model for this principle by introducing a message passing neural network which can directly consume heterogeneous multimodal data, represented as knowledge graph, and which itself can learn to extract relevant information from each modality, based solely on the downstream task.

We call a knowledge graph that contains information in multiple modalities a multimodal knowledge graph. The most elementary modality—the relational information—is encoded in the graph structure. Other common modalities are of numerical, textual, and temporal nature, such as various measurements, names, and dates, respectively, and, in a lesser degree, of visual, auditory, and spatial makeup. In a knowledge graph about monuments, for example, we might find that each monument has a detailed description, a registration number, a year in which it was build, a few pictures from different angles, and a set of coordinates (Figure 1). These and other attributes are encoded as raw values with a corresponding datatype declaration, called literals, and tell us something about the objects they are connected to, called entities. However, most of this information is lost when we reduce the literals to identifiers, as is currently common practice when we apply message passing networks to knowledge graphs.

By reducing literals to identifiers, we discard any information that is contained in their contents, retaining only the relational information encoded by their connections, and placing them on an equal footing with all other entities. This means that we are effectively feeding our models a subset of the original and complete knowledge, but also that we are depriving our models of the ability to compare inputs according to their modalities: measurements as numbers, descriptions as language, coordinates as geometries, etc. As a result, our models are unable to distinguish between literals that are closely together in the value space with those which are far apart. The name Mary, for example, would be seen as (dis)similar to Maria as it would to Wilberforce, as would the integer value 47 be to 42 and $6.26068 \times 10^{-34}$. Instead however, we want our models to use this information to guide their learning process.

By enabling our models to naturally ingest literal values, and by treating these values according to their modalities, tailoring their encodings to their specific characteristics, we stay much closer to the original and complete knowledge that is available to us. We believe that doing so enables our models to create better internal representations of the entities we are trying to learn over, potentially resulting in an increase in the overall performance of our models. In this work, we test this supposition by feeding information from many different modalities through dedicated (neural) encoders into a joint representation space by means of late fusion. By embedding our approach within the message passing framework, and by exploiting datatype declarations and common vocabularies such as XSD\(^2\) and OGC\(^3\), we embrace the idea that this enables us to learn end-to-end from any heterogeneous multimodal data, as long as they are represented as knowledge graph. To evaluate our supposition, we investigate the influence of each separate modality on the classification accuracy on six different heterogeneous multimodal knowledge graphs.

Because the interest in multimodal learning on knowledge graphs has emerged only recently, only few multimodal benchmark datasets exist, most of which only in-
clude numerical and textual information [7, 8]. Images are also often included, but are stored outside the graph and linked to using hyperlinks and imported during runtime. To add to this modest collection, we have created a knowledge graph about monumental buildings in the Netherlands that includes heterogeneous information from six different modalities, all of which are incorporated in the graph (see Sc. 5.2 for more details). We offer this dataset to the community with the hope that it can be used to further the research on this topic.

To summarize, the main contributions of this paper are:

1. A machine learning model, embedded in the message passing framework, which can learn end-to-end from any heterogeneous knowledge graph, and which can naturally ingest literal values according to their modalities.

2. An inverse ablation study on the potential usefulness of including information from multiple modalities, and the effect this has on the overall performance of our models.

3. A knowledge graph about monuments in The Netherlands which contains information from six different modalities, and which we offer as benchmark.

Our aim is emphatically not to show that our approach achieves any kind of state-of-the-art, or even to measure its performance against related models. For this purpose the available benchmark data is insufficiently mature. Rather, we present our approach as a proof-of-concept. We show that in certain cases, a model can be trained end-to-end on a heterogeneous knowledge graph so that it learns purely from the downstream classification task, which patterns to extract from each modality.

2 Related Work

Machine learning from multimodal sources is a well-studied problem. A good introduction to the problem and its many perspectives is given by [1]. According to their taxonomy, our approach is one of late fusion by message passing network, focusing on representation of multiple modalities in a joint representation space. We consciously ignore the hard problems of alignment and translation: data in a given modality is only every used to learn a vector representation of a literal node.

Various other approaches have explored using the information from literal nodes from one or more modalities in knowledge graph machine learning models. An overview is provided by [2] for the specific use case of link prediction. While two of the models surveyed, only MKBE [8] use literals representing a variety of modalities, including images. Like our approach, MKBE uses a set of modality specific (neural) encoders to map multimodal information to embedding vectors.

All these models are simple embedding models, based on a score function applied to triples. By contrast, our approach includes a message passing layer, allowing multimodal information to be propagated through the graph, several hops, before being used for classification.

Our model is currently only evaluated on entity classification, putting a direct comparison to these methods out of scope.

3 Preliminaries

Knowledge graphs and message passing neural networks are integral components of our research. We will here briefly introduce both concepts.

3.1 Knowledge Graphs

For the purposes of this paper we define a multimodal knowledge graph $G = (V, E)$ over modalities $M$ as a labeled multidigraph defined by a set of nodes $V = I \cup L$ and a set of directed edges $E$, and with $n = |V|$. Nodes belong to one of two categories: entities $I$, which represent objects (monuments, people, concepts, etc.), and literals $L$, which represent raw values in modality $m \in M$ (numbers, strings, coordinates, etc.). We also define a set of relations $R$ which contains the edge types that make up $E$. Relations are also called predicates.

Information in $G$ is encoded as triples $T$ of the form $(h, r, t)$, with head $h \in I$, relation $r \in R$, and tail $t \in I \cup L$. The combination of relations and literals are also called attributes or node features.

See Figure 1 for an example of knowledge graph with seven nodes, two of which are entities and the rest literals.
All knowledge graphs in this paper are stored in the Resource Description Framework format [6], but our model can be applied to any graph fitting the above definition.

3.2 Message Passing Neural Networks

A message passing neural network [3] is a graph neural network model that uses trainable functions to propagate node embeddings over the edges of the neural network. One simple approach to message passing is the graph convolutional neural network (GCN) [5]. The R-GCN [11], on which we build, is a straightforward extension to the knowledge graph setting.

Let $H^0$ be a $n \times q$ matrix of $q$ dimensional node embeddings for all $n$ nodes in the graph. That is, the $i$-th row of $H^0$ is an embedding for the $i$-th node in the graph.

The R-GCN computes an updated $n \times l$ matrix $H^1$ of $l$-dimensional node embeddings by the following computation (the graph convolution):

$$H^1 = \sigma \left( \sum_{r \in \mathcal{R}} A^r H^0 W^r \right)$$

Here, $\sigma$ is an activation function like ReLU, applied element-wise. $A^r$ is the row-normalised adjacency matrix for the relation $r$ and $W^r$ is a $q \times l$ matrix of learnable weights. This operation arrives at a new node embedding for a node by averaging the embeddings of all its neighbours, and linearly projecting to $l$ dimensions by $W^r$. The embeddings are then summed over all relations and a non-linearity $\sigma$ is applied.

To use R-GCNs for entity classification with $c$ classes, the standard approach is to start with one-hot vectors as initial node embeddings (that is, $H^0 = I$). These are transformed to $h$-dimensional node embeddings by a first R-GCN layer (commonly with $h = 16$), which are transformed to $c$-dimensional node embeddings by a second R-GCN layer. The second layer has a row-wise softmax non-linearity, so that the final node embeddings can be read as class probabilities. The network is then trained by computing the cross-entropy loss for the known labels and backpropagating to update the weights. Using more than two layers of message passing does not commonly improve performance with current message passing models.

To allow information to propagate in both directions along an edge, all inverse relations are added to the predicate set. The identity relation is also added (for which $A^r = I$) so that the information in the current embedding can, in principle, be retained. To reduce overfitting, the weights $W^r$ can be derived from a smaller set of basis weights by linear combinations (see the original paper for details).

4 A Multimodal Message Passing Network

We introduce our model as an extension to message passing networks which can learn end-to-end from the structure of an arbitrary graph, and for which holds that $H^0 = I$. To do so, we let $f(\cdot)$, $g(\cdot)$, and $h(\cdot)$ be feature encoders that output feature embeddings of lengths $\ell_f$, $\ell_g$, and $\ell_h$ for nodes $v_i \in \mathcal{V}$. We define $\mathbf{F}$ as the $n \times f$ matrix of multimodal feature embeddings with $f = \ell_f + \ell_g + \ell_h$, and concatenate $\mathbf{F}$ to the identity matrix $I$ to form multi-
modal node embeddings:

\[ H^0 = [I \ F] \]

of size \( n \times q \) (Fig. 2).

Embedding matrix \( H^0 \) is fed together with \( A^r \) to a message passing network, such as the R-GCN. Both encoders and network are trained end-to-end in unison by backpropagating the error signal from the network through the encoders all the way to the input.

4.1 Modality Encoders

We add encoders for five different modalities which are commonly found in knowledge graphs. We forgo discussing relational information—the sixth modality—as that is already extensively discussed in related work on message passing networks. For numerical and temporal information, we use straightforward deterministic encodings due to the simplicity of the problem. For textual, visual, and spatial information we use neural encoders, for which we chose convolutional neural networks (CNN) because of their efficiency and speed. In the case of neural encoders, we also introduce an intermediate step in which we convert the raw values to their vector representations.

In the following, we let \( e_i^m \) be the feature embedding vector of node \( v_i \) for modality \( m \). The concatenation of a node’s identity vector and all its feature embedding vectors \( e_i^m \) for every \( m \in \mathcal{M} \) equals the \( i \)-th row of \( H^0 \).

4.1.1 Numerical Information

Numerical information encompasses the set of real numbers \( \mathbb{R} \), and corresponds to literal values with a datatype declaration of XSD:double, XSD:float, and XSD:decimal and any subtype thereof. For these, we simply take the values themselves as their embeddings, and represent these in a shared embedding space. We also include values of the type XSD:boolean into this category due to lack of a more faithful representation, but separate their embeddings from those of real numbers to convey a difference in semantics.

More concretely, for all nodes \( v_i \in \mathcal{V} \) holds that \( e_i^{\text{numerical}} \) is the concatenation of their numerical and boolean components, encoded by functions \( f_{\text{num}} \) and \( f_{\text{bool}} \), respectively. Here, \( f_{\text{num}}(v_i) = v_i \) if \( v_i \) is a literal node with a value in \( \mathbb{R} \). If \( v_i \) is a boolean instead, we let \( f_{\text{bool}}(v_i) = 1.0 \) if \( v_i \) is \text{true} and \( -1.0 \) if \( v_i \) is \text{false}. In both cases, we represent missing or erroneous values with \( 0.0 \) (we assume a normalization between -1 and 1).

4.1.2 Temporal Information

Literal values with datatypes which follow the Seven-property model\(^5\) such as XSD:time, XSD:date and XSD:gMonth, are treated as temporal information. Different from numerical values, temporal values contain elements that are defined in a circular value space and which should be treated as such. For example, it is incorrect to say that January and December are \textit{always} 11 months apart, as would be implied by directly feeding the months’ number to our models. Instead, it is more accurate to encode this as

\[ f_{\text{trig}}(\phi, \psi) = [\sin\left(\frac{2\pi \phi}{\psi}\right), \cos\left(\frac{2\pi \phi}{\psi}\right)] \]

with \( \psi \) the number of elements in the value space (here 12), \( \phi \) the integer representation of the element we want to encode, and \( f_{\text{trig}} \) a trigonometric function in our encoder.

We use this encoding for all other circular elements, such as hours (\( \psi = 24 \)) and decades (\( \psi = 10 \)). When dealing with years however, we decided to encode smaller changes more granular than larger changes. That is, years are split into centuries, decades, and (single) years fragments, with decades and years treated as circular elements but with centuries as numerical values (we limit our domain to years between \( -9999 \) and \( 9999 \)).

Concretely, consider date literals of the form (\(+\-\)YYYY-MM-DD) (we omit timezone specification for simplicity). For every node \( v_i \) of this form we let \( e_i^{\text{temporal}} \) be 1.0 and \(-1.0\) at index \( j \) for CE and BCE, respectively, \( e_i^{\text{temporal}} \) at index \( k \neq j \) the centuries in \( \mathbb{N} \), and with decades, (single) years, months, and days represented as in Equation 3, resulting in an embedding of length 10.

4.1.3 Textual Information

Vector representations for textual attributes with the datatype XSD:string or any subtype thereof, are created using a character-level encoding, proposed in [16].

\(^5\)https://www.w3.org/TR/xmlschema11-2
Hereto, we let $E^s$ be a $|\Omega| \times |s|$ matrix representing string $s$ using vocabulary $\Omega$, such that $E^s_{ij} = 1.0$ if $s_j = \Omega_i$, and 0.0 otherwise.

A character-level representation enables our models to be language agnostic and independent of controlled vocabularies (allowing it to cope with colloquiums and identifiers for example), as well as provide some robustness to spelling errors. It also enables us to forgo the otherwise necessary stemming and lemmatization steps, which would remove information from the original text. The resulting embeddings are optimized by running them through a temporal CNN $f_{\text{char}}$ with output dimension $c$, such that $e^\text{textual}_i = f_{\text{char}}(E^\text{vi})$ for every node $v_i$ with a textual value.

### 4.1.4 Visual Information

Images and other kinds of visual information (e.g. videos, which can be split in frames) can be included in a knowledge graph by either linking to them or by expressing them as binary string literals with the datatype `XSD:b64string` which are incorporated in the graph itself (as opposed to storing them elsewhere). In either case, we first have to obtain the raw image files by downloading and/or converting them.

Let $im_i$ be the raw image file as linked to or encoded by node $v_i$. We can represent this image as a tensor $E^{im_i}$ of size `channels x width x height`, which we can feed to a two-dimensional CNN $f_{im}$ with output dimension $c$, such that $e^{\text{visual}}_i = f_{im}(E^{im_i})$ for the image associated with node $v_i$.

### 4.1.5 Spatial Information

Spatial information includes points, polygons, and any other spatial features that consist of one or more coordinates. These features can represent anything from real-life locations or areas to molecules or more abstract mathematical shapes. Literals with this type of information are typically expressed using the well-known text representation (WKT) and therefore carry the `OGC:wktLiteral` datatype declaration. The most elementary spatial feature is a coordinate (point geometry) in a $d$-dimensional space, expressed as `POINT(x_1 \ldots x_d)`, which can be combined to form more complex types such as lines and polygons.

We use the vector representations proposed in [14] to represent all supported spatial features as the enumeration of their coordinates. Let $E^{sf}$ be the $|x| \times |sf|$ matrix representation for spatial feature $sf$ consisting of $|sf|$ coordinates, and with $x$ the vector representation of one such coordinate. Vector $x$ holds all of the coordinate’s $d$ points, followed by its other information (e.g. whether it is part of a polygon) encoded as binary values. For spatial features with more than one coordinate, we also need to separate their location from their shape to ensure that we capture both these components. To do so, we encode the location in $\mathbb{R}^d$ by taking the mean of all coordinates that makeup the feature. To capture the shape, we compute the global mean of all spatial features in the graph, and subtract this from their coordinates to place their centre around the origin.

We optimize the vector representations using a temporal CNN $f_{sf}$ with output dimension $c$, such that $e^{\text{spatial}}_i = f_{sf}(E^{vi})$ for all nodes $v_i$ which express spatial features.

### 5 Experiment

We evaluate our model on an entity classification task while varying the modalities which are included in the learning process. To do so, we compute the classification accuracies for each combination of structure and modality, as well as all modalities combined, and evaluate this against using only the relational information and the performance on a majority class classifier.

Another dimension that we test is how a graph’s structure is represented and fed to our model, and how this influences the performance with and without node features. The two graph representations that we test on differ only in how they deal with literal nodes that have the same value. The most common approach is to collapse these literals into a single node, which we will refer to as merged literals, whereas the alternative is to keep these duplicate values separated and represent them by as many nodes as there are values. We will call this latter configuration the split literals.

#### 5.1 Implementation

For our implementation\(^5\), we use the R-GCN as main building block onto which we stack our various encoders.
The R-GCN can learn end-to-end on the structure of relational graphs, taking relational types into account, and which is therefore a suitable choice to learn on knowledge graphs. If we are only interested in learning from a graph’s structure, we let \( H^0 \) be the nodes’ \( n \times n \) identity matrix \( I \). (that is, \( H^0 = I \)). To also include literal values in the learning process, or node features, we let \( F \) be the \( n \times f \) feature embedding matrix and concatenate this to \( H^0 \) as in Equation 2 to form \( H^0 = [I \ F] \). To cope with the increased complexity brought on by including node features we optimize our implementation for sparse matrix operations by splitting up the computation of Equation 1 into the sum of the structural and feature component. For this, we once again split \( H^0 \) into identity matrix \( H_I = I \) and feature matrix \( H^0_F = F \), and rewrite the computation as

\[
H^1 = \sigma \left( \sum_{r \in \mathcal{R}} A^r H_I W^r_I + A^r H^0_F W^r_F \right) \quad (4)
\]

Here, \( W^r_I \) and \( W^r_F \) are the learnable weights for the structural and feature components, respectively. For layers \( i > 0 \) holds that \( H^i_I = H^1 \), and that \( A^r H^i_I W^r_I = 0 \). Note that because \( A^r H_I = A^r \), we can omit this calculation when computing Equation 4, and thus also no longer need \( H_I \) as input. Figure 3 illustrates this computation as matrix operations.

### 5.1.1 Neural Encoders

All three neural encoders are implemented using CNNs. For textual information, we use a temporal CNN with 4 convolutional layers, each followed by ReLU, and 3 dense layers (Table 1), which has a minimal input sequence length of 12 characters. A similar setup is used for the spatial encoder, but with 3 convolutional layers and with a different number of filters (Table 2), and with a minimal input length of 4 coordinates. In both cases, we trim outliers and use zero padding where needed. For the visual encoder, we use the efficient MobileNets architecture from [4], with an output dimension of 128. All three CNNs are initiated using \( \mathcal{N}(0, 1) \), and are trained using mini batching (4 passes per epoch).

The output of layer \( i \) from all encoders for all nodes in \( V \) are concatenated to form \( H^i_F \), which is passed to Equation 4 together with \( A^r \). A final row-wise softmax non-linearity is added to output class probabilities.

### 5.2 Datasets

We evaluate our model on six knowledge graphs with different degrees of multimodality. General and modality-specific statistics about each of these are listed in Table 3 and 4, respectively.

AIFB, MUTAG, BGS, and AM are existing benchmark datasets for machine learning on knowledge graphs [10]. However, AIFB, BGS, and AM lack the datatype declarations needed to accurately determine the literals’ modalities, which were therefore added by us to create the AIFB+, BGS+, and AM2D+ datasets. AM2D+ further differs from AM in that we added images, and that we pruned the graph to include only the nodes up to depth two from the labeled entities (due to the practical difficulties caused by the increased size).

A fifth dataset, the Dutch Monument Graph (DMG), was compiled by us as benchmark for multimodal learning on knowledge graphs, and includes information from all five modalities listed in Section 4.1, in addition to the relational information encoded by the graph’s structure. The graph integrates three existing public knowledge graphs published by the Dutch Cultural Heritage

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6Code available at https://gitlab.com/wxwilcke/mrgcn

7Datasets available at https://gitlab.com/wxwilcke/mmkg
Table 1: Configuration of the textual encoder with 4 convolutional layers (top) and 3 dense layers (bottom). For pooling layers, Max(k/s) lists kernel size (k) and stride (s), or Max(·) when it depends on the input sequence length.

| Layer | Filters | Kernel | Padding | Pool     |
|-------|---------|--------|---------|----------|
| 1     | 64      | 7      | 3       | Max(2/2) |
| 2     | 64      | 7      | 3       | Max(2/2) |
| 3     | 64      | 7      | 3       | -        |
| 4     | 64      | 7      | 2       | Max(·)   |

| Layer | Dimensions |
|-------|------------|
| 5     | 256        |
| 6     | 64         |
| 7     | 16         |

Table 2: Configuration of the spatial encoder with 3 convolutional layers (top) and 3 dense layers (bottom). For pooling layers, max(k/s) lists kernel size (k) and stride (s), whereas avg(·) depends on the input sequence length.

| Layer | Filters | Kernel | Padding | Pool     |
|-------|---------|--------|---------|----------|
| 1     | 16      | 5      | 2       | max(3/3) |
| 2     | 32      | 5      | 2       | -        |
| 3     | 64      | 5      | 2       | avg(·)   |

| Layer | Dimensions |
|-------|------------|
| 4     | 128        |
| 5     | 32         |
| 6     | 16         |

6 Results & Discussion

The results are listed in Table 5 and 6 for merged and split literal configurations, respectively, and report the average classification accuracy over 10 runs on the test sets. For DMG and SYNTH, these sets were created using the 80/20/20 rule, whereas for the others we used the splits from [10]. For each dataset, we show the results for learning with and without node features, as well as a breakdown per modality if available. All results were obtained using a two-layer R-CGN with 16 hidden nodes, and were trained in full batch mode with Adam for 100 epochs with early stopping (after no improvement for 7 epochs) and with an initial learning rate of 0.01. Note that all results are with respect to those of learning using just the graph’s structure, which serves as our baseline.

The overall results show a small to considerable improvement when including certain node features for almost all datasets, except for AM2D+ of which the difference might also be due to randomness in initialization. However, any difference in performance seems to depend strongly on which modality we include: some modalities improve the baseline by little to nothing, whereas others improve or worsen it considerably. These differences appear to stack when we include information from all supported modalities, with the best or worst modality pulling or dragging the combined results up or down, respectively. The results on SYNTH seem to indicate that at least part of this is caused by the particular characteristics.
Table 3: Datasets used in our experiments. The AIFB+, AM2D+, and BGS+ datasets were extended with datatype declarations, and images were added to the AM+ dataset. Literals with the same value are counted as the same node in the merged count, whereas they are counted separately in the split count.

| Dataset | AIFB+ | SYNTH | DMG | MUTAG | AM2D+ | BGS+ |
|---------|-------|-------|-----|-------|-------|------|
| Facts   | 29,219| 30,600| 51,179| 74,567| 639,190| 916,345|
| Relations| 45    | 38    | 37  | 23    | 123   | 103  |
| Labeled | 176   | 256   | 600 | 340   | 1000  | 146  |
| Classes | 4     | 2     | 6   | 2     | 11    | 2    |
| Entities (merged) | 6,072 | 5,976 | 25,557 | 32,621 | 174,401 | 258,519 |
| Literals (merged) | 5,468 | 20,274 | 15,080 | 1,104 | 258,222 | 230,790 |
| Entities (split) | 2,835 | 4,098 | 5,704 | 22,540 | 146,609 | 103,055 |
| Literals (split) | 8,705 | 22,152 | 34,933 | 11,185 | 53,614 | 386,254 |

Table 4: Distribution of datatypes in the datasets. Numerical information includes all subsets of real numbers, as well as booleans, whereas date, years, and other similar types are listed under temporal information. Textual information includes strings and its subsets, as well as raw URIs (e.g. links). Images and geometries are listed under visual and spatial information, respectively.

| Dataset | AIFB+ | SYNTH | DMG | MUTAG | AM2D+ | BGS+ |
|---------|-------|-------|-----|-------|-------|------|
| Numerical | 115 | 7,382 | 1,342 | 11,185 | 11,113 | 12,332 |
| Temporal | 1,227 | 3,727 | 219 | - | 14,798 | 13 |
| Textual | 7,363 | 3,701 | 29,044 | - | 26,891 | 279,940 |
| Visual | - | 3,652 | 3,279 | - | 812 | - |
| Spatial | - | 3,690 | 1,049 | - | - | 73,870 |
| Other | - | - | - | - | - | 20,098 |

of the datasets, such as noisy signals from semi-random or task-irrelevant attributes (e.g. identifiers). However, our models should learn to ignore these signals, which might indicate another cause, for instance because the weights of the neural encoders are shared for all attributes of the same modality despite the different domains of properties that makeup that modality.

We can also see a difference depending on whether or not we merge literal values, with an overall similar or lower performance when we split literals. The results on SYNTH seem to indicate that this difference—0.69 vs. 0.50 on baseline—can be attributed to information from literal values being encoded in the graph’s structure, which suggests that explicitly including additional modalities may not always be worth the increased complexity as the information is already implicitly present in the graph. This is supported by the difference between the majority class and the baseline results, which shows how much of the signal exactly is captured in the relational information. Nevertheless, on datasets where only little or no signal is present in the structure, such as SYNTH and DMG, including information from other modalities appears to increase the performance significantly (except for MUTAG, which might be caused by the low ratio of literals to entities).

Finally, we must note the poor results with spatial features on SYNTH, despite providing a slight gain and drop in performance for DMG and BGS, respectively. As the results on SYNTH are even below that of the majority class, we believe that this is a problem of how we generated the spatial features, rather than an indication that including spatial information should be avoided.
Table 5: Entity classification results in accuracy, averaged over 10 runs, with only unique literals (merged configuration). Structure uses only the relation information whereas Structure + Features also includes information from all supported modalities. The rest provides a breakdown per modality.

| Dataset        | AIFB+ | SYNTH | DMG  | MUTAG | AM2D+ | BGS+ |
|----------------|-------|-------|------|-------|-------|------|
| Majority Class | 0.4167| 0.5000| 0.1667| 0.6618| 0.3333| 0.6552|
| Structure      | 0.9583| 0.6942| 0.5917| 0.6956| 0.8803| 0.8242|
| Structure + Features | 0.8861 | 0.8173 | 0.7324 | 0.8399 | 0.8414 |
| Structure + Numerical | 0.9583 | 0.7500 | 0.5958 | 0.7324 | 0.8773 | 0.8414 |
| Structure + Temporal | 0.9666 | 0.7981 | 0.5767 | -     | 0.8694 | 0.8242 |
| Structure + Textual | 0.9139 | 0.6952 | 0.7317 | -     | 0.8152 | 0.8276 |
| Structure + Visual | -    | 0.9250 | 0.4042 | -     | 0.8187 | -    |
| Structure + Spatial | -   | 0.4962 | 0.6233 | -     | -     | 0.7552 |

Table 6: Entity classification results in accuracy, averaged over 10 runs, with literals with the same value are kept separately (split configuration). Structure uses only the relation information whereas Structure + Features also includes information from all supported modalities. The rest provides a breakdown per modality.

| Dataset        | AIFB+ | SYNTH | DMG  | MUTAG | AM2D+ | BGS+ |
|----------------|-------|-------|------|-------|-------|------|
| Majority Class | 0.4167| 0.5000| 0.1667| 0.6618| 0.3333| 0.6552|
| Structure      | 0.9167| 0.5019| 0.2308| 0.6559| 0.8561| 0.8414|
| Structure + Features | 0.8611 | 0.7462 | 0.4850 | 0.6721 | 0.8394 | 0.8449 |
| Structure + Numerical | 0.9167 | 0.6558 | 0.3096 | 0.6721 | 0.8583 | 0.8414 |
| Structure + Temporal | 0.9167 | 0.7442 | 0.2350 | -     | 0.8593 | 0.8380 |
| Structure + Textual | 0.7611 | 0.7039 | 0.5456 | -     | 0.8182 | 0.8276 |
| Structure + Visual | -    | 0.8981 | 0.2508 | -     | 0.8515 | -    |
| Structure + Spatial | -   | 0.4558 | 0.2433 | -     | -     | 0.8276 |

7 Discussion

In this work, we have introduced a model for end-to-end multimodal learning on heterogeneous knowledge graphs which treats literals as first-class citizen by encoding them in accordance with the characteristics of their modalities.

Our results indicate that, overall, including information from other modalities can improve the performance of our models either slightly or considerably, depending strongly on the characteristics of the data and whether or not we merge literals with the same value (thereby encoding literal information in the structure of the graph). We believe that these results support our supposition that by including as much information as possible, staying closer to the original and complete information in the graph, enables our models to learn better internal representations of its nodes, with an overall increase in performance as result. Nevertheless, more research is needed to understand how we can best include multimodal node features in the learning process.

7.1 Limitations and future work

Our aim has currently been to demonstrate that we can train a multimodal message passing model end-to-end which can exploit the information contained in a graph’s literals and naturally combine this with its relational counterpart, rather than to established that our approach reaches state-of-the-art performance, or even to measure its performance relative to other published models.
To properly establish which type of model architecture performs best in multimodal settings, and whether message passing models provide an advantage over more shallow embedding models without message passing, we require more extensive, high-quality, standard benchmark datasets with well-defined semantics (i.e. datatype and/or relation range declarations). To this end, we have contributed the DMG knowledge graph, which contains literal nodes from various modalities. We have also contributed variants of three existing benchmark datasets, which we made suitable for multimodal learning by adding the necessary datatype declarations (and in one case also images). Nevertheless, to determine precisely what kind of data is most fitting for this form of learning we are likely to require an iterative process where each generation of models provides inspiration for the next generation of benchmark datasets and vice versa.

We also note that all knowledge graphs currently used in entity classification (including DMG) have a limited amount of labeled entities. This means that there is likely a large amount of variance in the estimated accuracies. To robustly establish best practices for model architectures, benchmark datasets with test sets of at least 10,000 entities will eventually be required. Our effort to generate a synthetic benchmark dataset which we can tweak as we wish might be a step in the right direction, although real-life data is much preferred.

So far we have only tested our method on entity classification, as that is where the message passing aspect of the R-GCN seems to make the most difference. It is yet to be established whether this approach can also yield a performance benefit in the setting of link prediction—a question we are currently exploring. Note that any score function from the embedding methods in [2] can, in principle, be combined with the R-GCN layers and the encoders. This leads to a large configuration space of possible models. We reiterate that the first thing that is required to explore this space effectively is high-quality benchmark data.

We performed little hyperparameter tuning in our model development, since the aim was not to tune a model to optimal performance, but only to show that information from literal nodes could, in principle, benefit performance. Due to the exploratory nature of the project, the test set was used for evaluation multiple times during development. In future work, a more rigorous protocol will be followed, to avoid the effects of multiple testing.

Future work will also investigate the trade off between potentially improving the performance by using a separate set of learnable weights per relation (as opposed to sharing weights amongst literals of the same modality) and the complexity this would add. Another promising angle is to explore techniques to reduce the overall complexity of a multimodal model: the necessity of full batch learning with many message passing networks—a known limitation—makes it challenging to learn from large graphs; a problem which becomes even more evident as we start adding multimodal node features.

Lastly, a promising direction of research is the use of pretrained encoders. In our experiments, we show that the encoders receive enough of a signal from the downstream network to learn a useful embedding, but this signal is complicated by the message passing head of the network, and the limited amount of data. Using a modality-specific, pretrained encoder, such as GPT-2 for language data [9] or Inception-v4 for image data [13], may provide us with good general-purpose feature at the start of training, which can then be fine-tuned to the specifics of the domain.

### 7.2 Conclusion

Learning end-to-end on heterogeneous data has a lot of promise which we have only scratched the surface of. A model that learns in a purely data-driven way to use information from different modalities, and to integrate such information along known relations, has the potential to allow practitioners a much greater degree of hands-free machine learning on multimodal heterogeneous data.

We hope that our proof-of-concept serves as an inspiration, and will lead not only to further experimentation in model configurations, but also to the development of larger and even higher-quality benchmark datasets which are reflective of real-world use cases.

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\(^9\)https://www.triply.cc
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