

Degree Project in Computer Science and Engineering
Second cycle, 30 credits

Lightweight Memory Networks for Link Prediction

Generalization of the LiMNet Architecture

TITOUAN MAZIER

Lightweight Memory Networks for Link Prediction

Generalization of the LiMNet Architecture

TITOUAN MAZIER

Master's Program, Computer Science

Date: May 23, 2025

Supervisors: Šarūnas Girdzijauskas and Lodovico Giaretta

Examiner: Viktoria Fodor

School of Electrical Engineering and Computer Science

Host company: RISE, Research Institute of Sweden

Swedish title: Lightweight Memory Networks för Länkprediktion

Swedish subtitle: Generalization av LiMNet Arkitektur

Abstract

- User-item recommendation is a central problem for search engines, social
 medias and streaming services. Yet, it is challenging because it necessitate
 to deal with information that is both relational and evolving over time.
 And common solutions have commonly been neglecting one of these
 aspects.
- In this work, we try to address these limitations by using the recent Lightweight Memory Networks (LiMNet). A model that captures causal relationships within temporal interaction.
- We demonstrate the potential of this solution throughout a framework for user-item recommendation that allow us to compare the performance of LiMNet with other baselines. The datasets used for the experiments record edits on Wikipedia pages, edits on Reddit pages and music streams on LastFM website. Each of these dataset presenting different scales and challenges for user-item recommendation.

An abstract is (typically) about 250 and 350 words (1/2 A4-page) with the following components:

- What is the topic area? (optional) Introduces the subject area for the project.
- Short problem statement
- Why was this problem worth a Bachelor's/Master's thesis project? (i.e., why is the problem both significant and of a suitable degree of difficulty for a Bachelor's/Master's thesis project? Why has no one else solved it yet?)
- How did you solve the problem? What was your method/insight?
- Results/Conclusions/Consequences/Impact: What are your key results/ conclusions? What will others do based on your results? What can be done now that you have finished that could not be done before your thesis project was completed?

Keywords

Graph Representation Learning, Temporal Interaction Networks, Link Prediction, Data Mining, Machine Learning, Recommendations

Sammanfattning

Inside the following scontents environment, you cannot use a includefilename as the command rather than the file contents will end up in the for DiVA information. Additionally, you should not use a straight double quote character in the abstracts or keywords, use two single quote characters instead.

Alla avhandlingar vid KTH måste ha ett abstrakt på både engelska och svenska. Om du skriver din avhandling på svenska ska detta göras först (och placera det som det första abstraktet) - och du bör revidera det vid behov.

If you are writing your thesis in English, you can leave this until the draft version that goes to your opponent for the written opposition. In this way, you can provide the English and Swedish abstract/summary information that can be used in the announcement for your oral presentation. If you are writing your thesis in English, then this section can be a summary targeted at a more general reader. However, if you are writing your thesis in Swedish, then the reverse is true – your abstract should be for your target audience, while an English summary can be written targeted at a more general audience. This means that the English abstract and Swedish sammnfattning or Swedish abstract and English summary need not be literal translations of each other.

Do not use the glspl{} command in an abstract that is not in English, as my programs do not know how to generate plurals in other languages. Instead, you will need to spell these terms out or give the proper plural form. In fact, it is a good idea not to use the glossary commands at all in an abstract/ summary in a language other than the language used in the acronyms.tex file - since the glossary package does not support use of more than one language.

The abstract in the language used for the thesis should be the first abstract, while the Summary/Sammanfattning in the other language can follow

Nyckelord

Graph Representation Learning, Temporal Interaction Networks, Link Prediction, Data Mining, Machine Learning, Recommendations

Acknowledgments

It is nice to acknowledge the people that have helped you. It is also necessary to acknowledge any special permissions that you have gotten – for example, getting permission from the copyright owner to reproduce a figure. In this case, you should acknowledge them and this permission here and in the figure's caption. Note: If you do not have the copyright owner's permission, then you cannot use any copyrighted figures/tables/.... Unless stated otherwise all figures/tables/...are generally copyrighted.

I detta kapitel kan du ev nämna något om din bakgrund om det påverkar rapporten på något sätt. Har du t ex inte möjlighet att skriva perfekt svenska för att du är nyanländ till landet kan det vara på sin plats att nämna detta här. OBS, detta får dock inte vara en ursäkt för att lämna in en rapport med undermåligt språk, undermålig grammatik och stavning (t ex får fel som en automatisk stavningskontroll och grammatikkontroll kan upptäcka inte förekomma) En dualism som måste hanteras i hela rapporten och projektet

Stockholm, May 2025 Titouan Mazier

vi | Acknowledgments

Contents

1.	Introduction	1
	1.1. Purpose/Motivation	1
	1.2. Problem	2
	1.3. Goals	2
	1.4. Delimitation	2
	1.5. Contribution	2
	1.6. Ethics and Sustainability	2
2.	Background	3
	2.1. User-Item Link Prediction	
	2.2. Graph Representation Learning	4
	2.3. Dynamic Graphs	
	2.4. Cross-RNN	
	2.5. LiMNet	8
3.	Method	9
	3.1. Datasets	9
	3.2. Experimental framework	. 10
	3.2.1. Preparation of the data	. 11
	3.2.2. Batching Strategy	
	3.2.3. Training and evaluation loops	. 12
	3.2.4. Comparison of the embeddings	. 12
	3.2.5. Code maintainability	. 13
	3.3. Adaptations of the Lightweight Memory Networks (LiMNet)	
	architecture	. 14
	3.3.1. Loss functions	. 14
	3.3.2. Addition of time features	. 14
	3.3.3. Normalization of the embeddings	. 15
	3.3.4. Stacking several LiMNet layers	. 15
	3.4. Exploration of the baselines	. 16
4.	Results	. 17
	4.1. Effects of the proposed improvements for LiMNet	
	4.2. Comparison with Jodie	
	4.3. Effect of the batching strategy	
Re	eferences	. 19

List of Figures

Figure 2.1	Architecture of LiMNet . User embeddings are indicated in	
	green and items embeddings in purple	. 8
Figure 3.1	Architecture of LiMNet with two layers	16

List of Tables	
Table 3.1 Details of the datasets.	10

Acronyms and Abbreviations

- *CTDG* Continuous-Time Dynamic Graph: Dynamic graph were each edge is associated with a timestamp. 5, 6
- *GNN* **Graph Neural Networks**: Specialized neural networks that are designed for tasks whose inputs are graphs. 5
- *GRL* **Graph Representation Learning**: The task of computing high level representation of graphs, subgraphs, nodes or edges. Used as inputs for Machine Learning algorithms. 4, 5
- *GRU* **Gated Recurrent Unit**: A type of recurrent neural network that simplifies the LSTM architecture by combining the forget and input gates into a single update gate. 7
- *LiMNet* Lightweight Memory Networks: A neural network architecture that focuses on efficient memory utilization and lightweight design for temporal interaction network embeddings computations. vii, ix, 2, 8, 9, 11, 14, 15, 16, 17, 18
- LSTM Long-Short Term Memory: A type of recurrent neural network designed to effectively learn and remember short and long-term dependencies in sequential data by using specialized memory cells and gating mechanisms. 7
- *NLP* Natural Language Processing: Field of Machine Learning aiming at automatically interpreting spoken and written languages. 5
- *RNN* Recurrent Neural Network: A neural network whose output depends on both the inputs and on the state of an internal memory that is updated with each input. 6, 7
- *Temporal Interaction Network*: Dynamic network were each interaction constitute a punctual edge, i.e. an edge with no duration. 6

xiv | Acronyms and Abbreviations

Chapter 1 Introduction

1.1. Purpose/Motivation

The rapid expansion of digital technology has resulted in the production of an overwhelming abundance of information, to the point that it is a challenge to find relevant and meaningful material among the multitude. To not only alleviate but also leverage this information overload, the interest have surged for search engines and recommendation systems. These two subjects share one common goal: filtering information. Among the many techniques that have emerged to tackle this task, content personalization has emerged as a significant factor. Instead of filtering the information in the same way for everyone, the systems will use the user's context: their search history, demographics, pasts interactions with the system, etc. to filter the information to display. Content personalization is the whole core of recommendation systems, but it is also very efficient for search engines. For example, the search for the term "football" should yield different results for a user interested in American football and a user interested in association football (soccer).

Content personalization can be represented as a single algorithm that accepts as input user related information and output an item from a catalog. In order to measure the performance of such an algorithm, we need to know what items would be relevant for each users. Gathering this information is costly, and sometimes even impossible. However, it is easy to collect user behaviors such as interaction with items, thus, content recommendation is commonly approximated to an interaction prediction task.

Interaction prediction is a self-supervised learning task where interactions are given as inputs to predict future interactions, that will themselves be added used for later inference. What sets this task apart from other self-supervised tasks is the relational aspect of the information used, each interaction explicitly connecting information with other interactions and the interacting elements. In addition, interaction order and temporality usually matters.

LiMNet is a simple Machine Learning model of a new kind that is designed to process interactions in a causal way, leveraging both relational information and the interactions order. This model proved it's performance at solving the task of botnet detection in IoT network, and has been designed in a modular and adaptive way that makes it easy to employ for different tasks. Given these promising results and that it is designed to exploit precisely the specific information that makes interaction prediction challenging, we believe that LiMNet can be an interesting solution to the interaction prediction task.

1.2. Problem

The driving research question for this work is the following:

"Can LiMNet perform well for interaction prediction?"

1.3. Goals

1.4. Delimitation

1.5. Contribution

1.6. Ethics and Sustainability

Chapter 2 Background

This chapter provide the background for the project. In Section 2.1 we provide an overview of link prediction and the classical solutions for the problem, in Section 2.2 we further develop the concept of graph embedding and some common methods to create them. Then in Section 2.3 we discuss the addition of a time dimension in graph-shaped data and the way it can be exploited, followed by a presentation of cross-RNN architectures in Section 2.4. Finally we present the model of interest for this work in Section 2.5 and why we believe that it is a relevant addition to the task of link prediction.

2.1. User-Item Link Prediction

Content personalization can commonly be represented as a link-prediction problem in a user-item graph. In such a graph, each user and each item is associated to a node. An item can be any kind of information the user is interested in. It could be web pages, music tracks, items in an e-commerce catalog, and so on... For each interaction a user has with the system, it registers as an edge in the graph. The goal of the personalization system is to find which item is the most relevant for a given user, which is the same as predicting which interaction should be added next in the graph.

A classical approach to that problem is to measure how close each item is to the user in the graph. Research in graph theory has provided us with a range of different ways to compute closeness between two nodes, such as measuring the shortest path connecting them, how many neighbors they share or how exclusive their common neighbors are.

In addition of the relationship between users and items, most real-world system provide rich information about the nature of each interactions, users, and items. For example, in a music streaming service, an interaction can have a type (stream, like, playlist add, ...), as well as a listening duration. While each song can have information attached about its genres, its length, and for users, their age, and their location. All of this information is typically processed by Machine Learning systems that provide reliable results

for numerical features. The challenge is then to meld traditional Machine Learning approaches for numerical features with graph-based methods for relational information.

Lichtenwalter et al. proposed to approach link prediction as a supervised Machine Learning problem, instead of scoring each edge, they try, given an edge, to predict if it will exist in the future. To include the relational data to their model, they add some of the closeness metrics discussed earlier to the users and items features[1]. This typical machine learning setup leads to switch from a straightforward prediction setting to a feature engineering approach when it comes to graph-based data. Instead of looking for the desired property in the structure of the graph, this approach will try to summarize the structure into rich representation compatible with machine learning algorithm. The goal is not to proxy the desired property, but to create a rich representation of the graph data that can be used by a machine learning algorithm.

All the previously mentioned methods presents one main drawback: each time a user want to be predicted an item, the score for each item regarding that user must be evaluated. This constraint makes it impossible to scale the solutions to large pools of items. To limit the number of comparisons, a solution is to create a high-dimensional representation of the users and items separately and use simple proximity functions on these embeddings as a scoring function. This spatial representation allow to reduce the problem to a nearest neighbor search for which scalable solutions have been found.

2.2. Graph Representation Learning

The task of learning high level representation from graph data is called Graph Representation Learning, abbreviated as GRL . GRL is a general subject in data mining, it can be used to classify graph structures such as protein graphs, to capture information from a subgraph for example by creating subgraph representation from a knowledge graph to feed into a Large Language Model. More commonly, GRL tries to create embeddings for nodes in a graph. These embeddings must capture information about the node's features but also about the context of the node in the graph, which is typically defined as the neighboring nodes and their respective features and context.

Two main approaches have emerged to create these embeddings, the first one is inspired by Natural Language Processing (NLP) and the second one from Computer vision. The first approach creates random walks along the graph and assimilate each node to a token, and each random walk to a sentence or a sample of text. This way, any methods that produce word embeddings can also be used to create nodes embeddings. This method can even be used to create embeddings for paths or subgraphs.

The second approach is inspired by convolutional networks used in computer vision. The idea is that convolutional networks see images as graphs of pixels and successively apply transformation to these pixels based on their direct neighborhood. Such operations can be applied similarly to general graphs, the main challenge being to accept neighborhood of varying size. These architectures are called Graph Neural Networks (GNN) and have proven very effective for GRL and link-prediction[2].

2.3. Dynamic Graphs

Most of the information we get from networks is dynamic, especially for user-item interaction networks where each interaction is usually happening at a given time. Yet, when dealing with relational data, this temporal dimension is often disregarded to limit the complexity of the problem, or simplified as a mere feature of the interaction. However temporal data constitute a unique kind of information, allowing to exploit causality relationship between the different interactions.

Causality is the idea that causes will have consequences in the future. It becomes especially critical when studying phenomenons that can spread through the networks like diseases, information, or trends. In such settings, each interaction can be the cause for a new state in the interacting nodes, requiring a different treatment for the same node at different times. While this concept is very intuitive for us, it is not the case for common GRL techniques described in Section 2.2 that let the information spread along the graph regardless of the order in which they are created.

In their review of dynamic network[3], Zheng et al. explain two ways temporal information are commonly included into graph data. The first one considers a series of snapshot of the graph at successive timestamps. The second one, called Continuous-Time Dynamic Graph (CTDG), records every edition to the graph as an event, associated with a timestamp. A typical event

in a CTDG is an edge addition or deletion. For this work, the focus is on CTDG with all events being punctual interactions. We call such networks Temporal Interaction Networks . These networks have the benefit to represent reality of a lot of system in a completely faithful way. However, the structure of the graph is blurry as each interaction corresponds to a point-in-time edge that is deleted as soon as it appears. Because of this, we tend to approach such graphs as a stream of interactions rather than a structured network.

A popular approach to leverage temporal data when creating nodes embeddings is to maintain a memory of the embeddings and update them as interactions are read. One of the building block for this approach is Deep-Coevolve[4], a model for link prediction that uses a cross-RNN (detailed further in Section 2.4) to update the representation of the users and items, followed by an intensity function to predict the best match for the user at every given time t. Following DeepCoevolve, other cross-RNN models have been proposed with notables performance upgrade.

JODIE[5] builds upon DeepCoevolve by adding a static embedding component to the representation, using the Cross-RNN part to track the users and items trajectories. It then employs a neural network layer to project the future embedding of each node at varying time. operation carried over by the intensity function in DeepCoevolve.

DeePRed[6] is an other approach building on top of DeepCoevolve, this time with the aim to accelerate and simplify the training by getting rid of the recurrence in the cross-RNN mechanism. To achieve this, the dynamic embeddings are computed based on static embeddings, effectively getting rid of the recurrence by never reusing the dynamic embeddings for further computations. The lack of long term information passing, is compensated by the use of a sliding context window coupled with an attention mechanism to best identify the meaningful interactions.

2.4. Cross-RNN

The key mechanism for all the aforementioned models is called cross-RNN where RNN stands for Recurrent Neural Network. A RNN is a neural network with the specificity of processing sequential data, passing an internal memory embedding between each step of the sequence of inputs. Formally, a RNN layer is defined as

$$o(i_t) = f(i_t, h_{t-1}) \tag{1}$$

$$\boldsymbol{h}_{t} = g(\boldsymbol{i}_{t}, \boldsymbol{h}_{t-1}) \tag{2}$$

Where t stands for the time step of the input i_t . $o(i_t)$ marks the output of the layer and h_t represent the memory of the layer after receiving the input i_t . The functions f and g can vary depending on the nature of the RNN but they will rely on weights, tuned during the model training. Popular RNN architectures try to keep a memory of long-term knowledge. Typically, the Long-Short Term Memory (LSTM) architecture maintains two distinct memories, a short term one and a long term one. The Gated Recurrent Unit (GRU) architecture iterate over LSTM by simplifying it, removing one of the two memories while keeping the gating mechanism. In practice both approaches perform significantly better than the naïve RNN implementation, with GRU achieving comparable performances than LSTM , in spite of its reduced cost.

A Cross-RNN layer is slightly different. Instead of keeping track of a single memory embedding \boldsymbol{h}_t , it maintain a memory for all nodes in the graph $\boldsymbol{H}_t = \left(\boldsymbol{h}_t^u\right)_{u \in \mathbb{U}} \cup \left(\boldsymbol{h}_t^i\right)_{i \in \mathbb{I}}$, where \mathbb{U} and \mathbb{I} are the sets of users and items in the graph. For each interaction (u,i,t,f) the memory is updated as follow:

$$\mathbf{h}_{t}^{u} = g^{u}(\mathbf{h}_{t-1}^{u}, \mathbf{h}_{t-1}^{i}, t, \mathbf{f})$$
(3)

$$\mathbf{h}_{t}^{i} = g^{i}(\mathbf{h}_{t-1}^{i}, \mathbf{h}_{t-1}^{u}, t, \mathbf{f})$$
(4)

And for all other users and nodes the memory is carried over.

$$\mathbf{h}_t^v = \mathbf{h}_{t-1}^v \qquad \forall v \in \mathbb{U} \setminus \{u\} \cup \mathbb{I} \setminus \{i\}$$
 (5)

Where u is the user interacting with item i at time t with feature f, and g^u and g^i are tunable functions, comparable to the function g in Eq. 2. LSTM and GRU cells designed for classical RNNs can be used for cross-RNN, the only modification being the memory management external to the cell.

The main benefit of cross-RNN architectures is that conservation of causality is granted by design. It comes, however, with a cost: the input of a cross-RNN model is sequential and cannot be made parallel. This cost is nonetheless mostly an issue for the training of the model, because processing one input in inference do not require to pass through the entire sequence.

2.5. LiMNet

LiMNet is a cross-RNN model designed to optimize the memory utilization and computational speed at inference time. In the original paper[7], LiMNet is designed as a complete framework for botnet detection in IoT networks, with four main components: an input feature map, a generalization layer, an output feature map and a response layer. For the purpose of this work, we will however consider LiMNet as a graph embedding module. Because the input feature map, output feature map and the response layer are task-dependent, the denomination "LiMNet" in this present work will designate only the generalization layer from this point.

LiMNet as a graph embedding module is a straightforward implementation of a cross-RNN module. This simplicity in the design brings two main benefits: first, LiMNet is very cheap to run at inference time, with a memory requirement linear in the number of nodes in the network. Secondly, it is flexible to node insertion or deletions. If a new node is added to the graph, it's embedding can be computed immediately, without a need to retrain the model. Node deletions are even easier to handle, all it takes is to delete the corresponding embedding from the memory. In practice, LiMNet has already proven it's potential on the task of IoT botnet detection[7] and fraud detection[8], it is thus expected that it could yield satisfying results for link-prediction, while requiring less resources than State of the Art solutions.

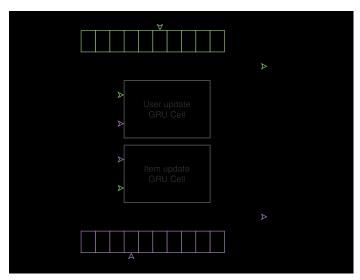


Figure 2.1: Architecture of LiMNet . User embeddings are indicated in green and items embeddings in purple.

Chapter 3 Method

In this chapter, we detail the experiments conducted throughout this work. First in Section 3.1, we introduce the datasets used in this work. Section 3.2 details the framework developed to conduct the experiments in a fair and controlled environment. Next, we present in Section 3.3 the various adaptations proposed for LiMNet to solve the task of link-prediction. Finally, we discuss in Section 3.4 exploration we conducted with the baselines.

3.1. Datasets

We use three public datasets in this project, all directly taken from the Stanford Large Network Dataset Collection (accessible at snap.stanford.edu/jodie/#datasets). More specifically, these datasets were created by Kefato et al. in [5] and have been reused a large number of time since then, to the point that they became informal standard benchmarks for interaction network predictions.

- Wikipedia edits: This dataset gathers edits on Wikipedia pages over the course of a month. It is made of the 1,000 most edited pages during the month and the 8,227 users that edited at least 5 time any of these pages. In total, the dataset records 157,474 edits.
- **Reddit posts:** This dataset was built in a similar fashion than the Wikipedia dataset. It comprises posts on the 1,000 most active subreddits, published by the 10,000 most active users over the course of a month. In total, this dataset records 672,447 interactions.
- **Reddit LastFM songs listens:** This dataset records music streams of the 1,000 most listened songs on the LastFM website. These streams are performed by 1,000 users throughout one month, and results in 1,293,103 total interactions.

The initial publication also included another dataset compiling user interaction with massive online open courses (MOOC). However, we decided to

set it aside because it contained too few data points to work with: only a couple interaction per users in average.

	Wikipedia	Reddit	LastFM
Users	8,227	10,000	1,000
Items	1,000	1,000	1,000
Interactions	157,474	672,447	1,293,103
Unique edges	18,257	78,516	154,993

Table 3.1: Details of the datasets.

The Table 3.1 summarizes the characteristics of the datasets. We can see that the main difference between the Wikipedia and the Reddit datasets is the density. They both have similar number of users and items but in Reddit there are about four times more connections between them than in Wikipedia. In LastFM the density is almost 20 times higher compared with Reddit, and the balance between users and items is also 10 time better. LastFM is therefore not only a bigger dataset but also a more challenging one to work with.

3.2. Experimental framework

Evaluating embedding models is a complex task because it requires to accommodate for a wide variety of inputs and outputs shapes, along with diverse training and inference procedures, while still ensuring the fairness of the evaluation between the different methods.

This complexity blooms with temporal graphs because there are different ways to approach them. One model can be approaching a temporal graph as a series of static graphs, another one can approach it as a time series [3], and yet another one could try to maintain a dynamical representation of the graph on the fly. None of this approach is inherently better or worse and they can all open different design opportunities.

In this section, we will precise the design decisions that led to our final evaluation framework. The implementation we came up with is publicly available at the following address: https://github.com/mazerti/link-prediction.

These decisions are grouped in four categories: Preparation of the data, Batching strategy, Training and evaluation loops, and comparison of the embeddings.

3.2.1. Preparation of the data

The datasets provide us with three types of information for each recorded interaction: the identifiers of the interacting user and item, the timestamp at which the interaction took place and a set of features providing additional information about the interaction. Most of the time, the models tested use only the identifiers and the implicit order of the interaction. Thus the framework will always provide as inputs the ids of the user and item interacting in the order the interactions happen.

In addition, the framework can add features to the inputs. These features can be requested either by the user through the configuration file, or directly by the model's implementation during the model's initialization. This second option allows to seamlessly add models relying on custom features without the requirement to manually request the features each time the model is used. This is especially relevant for time information, because each model can have a different use of the timestamps. A common usage is to use the time delta between successive interactions of a same user. This information would be expensive to compute at inference because it would require to keep track of the timestamp of the last interaction each user have performed at any time step. Pre-computing it as a feature on the other hand is much more convenient because we have access to all the interactions at once and computing time deltas results in a simple query operation.

3.2.2. Batching Strategy

As pointed out by previous work temporal interaction comes with a tradeoff regarding the ability to leverage parallelism for training. Kumar et al. proposed for their model JODIE an elaborate batching strategy based on the structure of the graph [5], and Kefato et al. removed the recursions from their model DeePRed by approximating the dynamic embeddings with static ones [6].

Inspired by the original LiMNet proposition [7], we decided instead to slice the data into sequences of fixed size. The idea is that big enough sequences could be good enough approximation of the actual sequence of all the interactions. While each sequence still require to be processed in order, several sequences can however be processed in parallel, speeding up the training.

3.2.3. Training and evaluation loops

The on-demand features preparation discussed in ensures that each model can access the inputs that it requires, unfortunately the models outputs also presents structural discrepancies. This work's scope is limited to embedding models, thus all model's outputs should be fixed size embeddings for either users or items. Some models, however, come with their own loss functions based on internal states, accessing the right outputs to compute either the loss function or the metrics from the embeddings is thus not something that can be managed identically for all models.

Because of this limitation, we made the decision to tie the evaluation logic of the models with the models implementations. This include going over a batch of interaction sequences, running the predictions, computing the loss, back propagation, updating the model memories, and producing measurable embeddings. However, we made sure to standardize all measures with fixed functions designed independently from the models with a sole purpose of measuring embeddings for the task of link prediction. In addition, we manage the training and evaluation loops in an unified way, limiting the risks of bugs due to errors in code reproduction. These loops include going over the batches, reporting the results, and iterating over the epochs,

3.2.4. Comparison of the embeddings

The next challenge in the implementation concerns the embeddings themselves. While we want to create embeddings to synthesize the information, it is not the actual end goal of the system. The end goal is to rank the items for a given user, and to rank the actual item the user will interact with high on the list. There are several ways to convert the embeddings into ranking, because this is not the focus of this work, we decided to use the most simple approach: to think of embeddings as points in a high dimension space and to rank the items embeddings by proximity with the user embedding. We did however consider two separate approaches to compute the proximity between embeddings.

The first one is to use the dot product of the normalized embeddings, which is equivalent to the cosine of the angle formed by the two embeddings with the origin of the embedding space.

$$dot_product_score(e^{user}, e^{item}) = \frac{e^{user}}{\|e^{user}\|} \cdot \frac{e^{item}}{\|e^{item}\|}$$
(6)

The higher the dot-product score between the user and an item embeddings, the closer these embeddings will be and thus the item should be ranked higher for that user.

The second proximity used is the L2 distance, a generalization of geometric distance to k-dimensional spaces.

$$L2_score(e^{user}, e^{item}) = \sqrt[k]{\|e^{user} - e^{item}\|^k}$$
 (7)

For this score, lower values will indicate closer embeddings and be ranked higher.

For all our experiments, we measure the performances with both scoring methods and report the higher value.

3.2.5. Code maintainability

For exploratory research projects such as this one, it is more efficient to write the whole code base from scratch rather than re-use an existing code base, because it remove from the research process the cruft of dependencies management, the need to understand the detail of the implementation as well as the necessity to comply with the existing framework. Getting rid of the existing also allow to approach problems from a different angle, and generally let the researcher focus on the novelty rather than the past. However, it is crucial to be able to reproduce experiments and to re-use existing models that can be used as baselines or as base for further developments.

Thus, this framework has been developed with the goal of being easy to understand and either build upon or reproduce. To reach this goal, two lines have been followed through the development process: thorough documentation and functional approach. The systematic documentations of every function in the framework should be able to help future researchers to understand the details of the implementation faster, whether it is for reusing it or to reproduce its behavior in a new experimental context. With the same goal of simplicity of understanding, the state have also been gathered as much as possible into a single location: the Context class. This class acts as a simple store for all stateful parts of the framework, making them never more than one variable away, wherever it is called from. In addition the framework has been written in a functional aspiring style, always favoring pure functions for their conceptual simplicity and consistency. Unfortunately this functional approach couldn't be applied on every part of the program, a

notable exception being the PyTorch modules that had to be implemented in an object oriented way to accommodate PyTorch's framework.

3.3. Adaptations of the LiMNet architecture

This work's primary goal was to test how the LiMNet model would perform for the link-prediction task. However, as discussed in Section 2.5, the implementation we use is stripped down of it's inputs and outputs maps, as well as the response layer used in the original paper to fit the specific needs of the task of IoT botnet detection.

3.3.1. Loss functions

We also had to adapt the loss used to train LiMNet because, unlike botnet detection, link-prediction isn't a classification setting so we couldn't use cross entropy Loss as the original model did. Instead we decided to use a mix of two losses. The first is an objective loss to minimize the distance between the embedding of the interacting user and item, it is calculated using the mean squared error for the embeddings or their dot product to 1. And the second is an regularization loss to maximize the information retention by maximizing the distance between different users and between different items. This loss is computed as follow:

$$L_{\text{reg}} = UU^T + II^T \tag{8}$$

Where U and I are respectively the matrix containing all the users embeddings and the matrix containing all the items embeddings.

In addition of this simplification, we tried to enhance the model with three separate additions: adding time features, normalizing the embeddings and stacking several LiMNet layers.

3.3.2. Addition of time features

While LiMNet take advantage of the order of the interaction to propagate information in a causal way, it doesn't use the actual timestamps to compute the embeddings. One of our assumption was that this would lead to a loss of relevant information that could otherwise have been useful to predict the best item. In order to check that assumption, we created time features to provide the model with information about when the interaction happen. We specifically intended to capture cyclic patterns in the user behaviors such as week/weekend or day/night differences in behaviors. Unfortunately, our

datasets only provide relative timestamps that obfuscated the exact time and day of the interactions, so we had to approximate these patterns by using a frequency decomposition of the timestamps. Specifically, we use the two following features:

$$\cos\left(\frac{2\pi}{\Delta_{\text{day}}}t\right), \sin\left(\frac{2\pi}{\Delta_{\text{day}}}t\right), \cos\left(\frac{2\pi}{\Delta_{\text{week}}}t\right), \sin\left(\frac{2\pi}{\Delta_{\text{week}}}t\right) \tag{9}$$

Where t is the timestamp of the interaction, and $\Delta_{\rm day}$ and $\Delta_{\rm week}$ are the duration of a day and a week in the unit of the timestamps. This aims at providing the model with a time representation that is more compatible with its machine learning components, that tend to fail to extract patterns from one dimensional values.

3.3.3. Normalization of the embeddings

An efficient way to compute the dot-product scores (Eq. 6) is to normalize all the embeddings to the unit sphere. While doing this, we realized that it could also be applied to the embeddings in LiMNet 's memory, this way, the cross-RNN mechanism is also fed with normalized embeddings as inputs. Our hopes were that this way the model would be more focus on encoding information through the angles between the embeddings rather than through their amplitudes.

Another benefit of this method is that it prevents the embeddings to collapse to 0. While the regularization loss is meant to prevent embeddings to converge all to the same value, it actually only make sure that the embeddings are not aligned, therefore, 0 remains a potential convergence point. Keeping the embeddings normalized at any time is therefore a good solution to that issue.

Our experiments yielded significantly better results with embeddings normalization, so we decided to use this modification by default for all the other experiments on LiMNet .

3.3.4. Stacking several LiMNet layers

The last improvement to LiMNet that we have tried was to stack several layers of the LiMNet architecture on top of each other, effectively turning it into a deep recurrent neural network. Figure 3.1 illustrate the architecture of

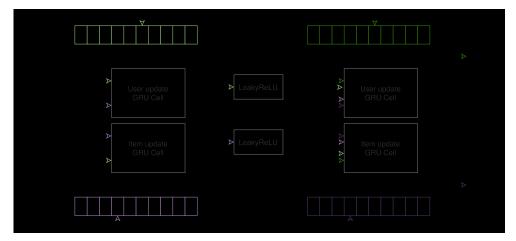


Figure 3.1: Architecture of LiMNet with two layers.

this new model. The leaky ReLU functions inserted in the middle have been added to create non-linearity and increase the expressiveness of the model.

3.4. Exploration of the baselines

We evaluated the performances of LiMNet against 2 other baselines: static embeddings and Jodie.

We trained static embeddings for each user and item, with the same loss functions that we described in Section 3.3.1 for LiMNet . This baseline is oblivious to the relational and temporal information contained in the data. It is also inconvenient to deploy for real world application because it requires to be entirely re-trained to account for any new information such as new interactions, new users, or new items.

The other baseline Jodie is described in [5], it is build upon the same core of cross-RNN embeddings than LiMNet but present three major differences. First, in addition to the dynamic embedding, Jodie uses one-hot representations of the users and items to create the embeddings. Secondly, Jodie exploits the time delta between two interaction of an user throughout a projection operation that tries to anticipate the embeddings' trajectory. Lastly, the model is trained with a dedicated loss function that ensure that the embeddings won't change too radically through an interaction. The difference between our implementation of Jodie and the original one lie in the absence of the t-batch algorithm, replaced by fixed-length sequences.

Chapter 4 Results

- Jodie is sensitive to the embedding size
- Adding layers to LiMNet doesn't improve the performance for link prediction
- Adding time features does not improve the performance
- Jodie can perform much better (???)
- Normalizing results seems to increase performances for LiMNet and Embeddings

Claim	Wikipedia		Reddit		Lastfm	
Changing embedding size Jodie	Ø	Ø	\checkmark	\checkmark	\checkmark	
Adding layers LiMNet	\checkmark	\checkmark	\checkmark	\checkmark	\checkmark	\checkmark
Adding time features LiMNet	\checkmark	\checkmark	\checkmark	\checkmark	\checkmark	~
Normalizing results LiMNet	\sim	~	\checkmark	\checkmark	\checkmark	\checkmark

• with little to no information the model is performing somewhat good

Experiments to conduct:

- · Each model at its best
- LiMNet with time features (none, both, day, week)
- LiMNet without normalization (with/without)
- LiMNet at several layers (1, 3, 5, 2)
- Jodie at several embedding size (32, 64, 16, 48, 128)
- Models with a small sequence length

In this chapter, we present the results of the **6** experiments performed. First, we discuss in Section 4.1 the measured performances of the proposed improvements on the LiMNet architecture. Then, Section 4.2 present the results yielded by our implementation of Jodie[5], and we discuss the differences we noticed with the initial publication. Lastly, Section 4.3 exhibits the impact of the batching strategy on the two models.

- 4.1. Effects of the proposed improvements for LiMNet
- 4.2. Comparison with Jodie
- 4.3. Effect of the batching strategy

References

- [1] R. N. Lichtenwalter, J. T. Lussier, and N. V. Chawla, "New perspectives and methods in link prediction," in *Proceedings of the 16th ACM SIGKDD International Conference on Knowledge Discovery and Data Mining*, in KDD '10. Washington, DC, USA: Association for Computing Machinery, 2010, pp. 243–252. doi: 10.1145/1835804.1835837.
- [2] Z. Wu, S. Pan, F. Chen, G. Long, C. Zhang, and P. S. Yu, "A Comprehensive Survey on Graph Neural Networks," *IEEE Transactions on Neural Networks and Learning Systems*, vol. 32, no. 1, pp. 4–24, 2021, doi: 10.1109/TNNLS.2020.2978386.
- [3] Y. Zheng, L. Yi, and Z. Wei, "A survey of dynamic graph neural networks," *Frontiers of Computer Science*, vol. 19, no. 6, p. 196323, Dec. 2024, doi: 10.1007/s11704-024-3853-2.
- [4] H. Dai, Y. Wang, R. Trivedi, and L. Song, "Deep Coevolutionary Network: Embedding User and Item Features for Recommendation," no. arXiv:1609.03675, arXiv, Feb. 2017. doi: 10.48550/arXiv.1609.03675.
- [5] S. Kumar, X. Zhang, and J. Leskovec, "Predicting Dynamic Embedding Trajectory in Temporal Interaction Networks," in *Proceedings of the 25th ACM SIGKDD International Conference on Knowledge Discovery & Data Mining*, in KDD '19. Anchorage, AK, USA: Association for Computing Machinery, 2019, pp. 1269–1278. doi: 10.1145/3292500.3330895.
- [6] Z. Kefato, S. Girdzijauskas, N. Sheikh, and A. Montresor, "Dynamic Embeddings for Interaction Prediction," in *Proceedings of the Web Conference 2021*, in WWW '21. Ljubljana, Slovenia: Association for Computing Machinery, 2021, pp. 1609–1618. doi: 10.1145/3442381.3450020.
- [7] L. Giaretta, A. Lekssays, B. Carminati, E. Ferrari, and S. Girdzijauskas, "LiMNet: Early-Stage Detection of IoT Botnets with Lightweight Memory Networks," in *Computer Security ESORICS 2021: 26th European Symposium on Research in Computer Security, Darmstadt, Germany, October 4–8, 2021, Proceedings, Part I,* in Lecture Notes in Computer Science. Springer Nature, 2021. doi: 10.1007/978-3-030-88418-5_29.

[8] Z. Cui, "Classification of Financial Transactions using Lightweight Memory Networks," 2022. [Online]. Available: https://urn.kb.se/resolve?urn=urn:nbn:se:kth:diva-321923