Internship Report

Paul LANDRIER
Supervised by Silviu Maniu

Contents

[TODO: Remove table of contents (it stays for now for better readability)]

abstract TODO (Mention broad usage of computation graphs (compilers)) Provenance-based method Paragraph in model is a good starting poitn

1 Introduction

TODO [Describe the interest of the computation]

2 Modeling a Computation

2.1 Computation Graphs

We try to abstract the notion of *computation graphs*, having in mind the particular example of neural networks.

Computation graphs are a type of graphs that represent a computation. Formally, in this work, we define a computation graph (V, E, Fun, Op) as a directed acyclic graph (V, E) together with a function $Fun : E \to F$ where F is a set of functions $S \to S$ (S is a fixed set, the same for all functions) and a function $Op : V \to Operator$ where $Operator$ is a set containing operators to aggregate several inputs in S. (Remark : usually in a computation graph, the functions are stored in the nodes and the edges represent a data dependency. We choose a different convention here to remain closer to provenance in

graphs as defined in [Ramusat, 2022]. For an other definition of computation graphs, see for instance [Wang and Zhao, 2023].)

For instance, if we want to compute the function $f(x) = e^{x^2}(x^2 + 2x + 2)$ using only the linear, "plus constant" and exponential functions, with + and × operators, then we can model a possible computation with the computation graph :

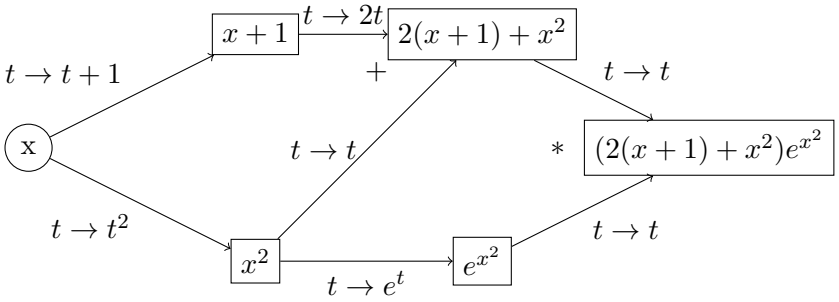


Figure 1: One possible computation graph of f.

Let's take the example of a (non-discretized) perceptron with two inputs. If we want to model its execution using only elementary operations and the activation function f, we get the representation in Figure 2.

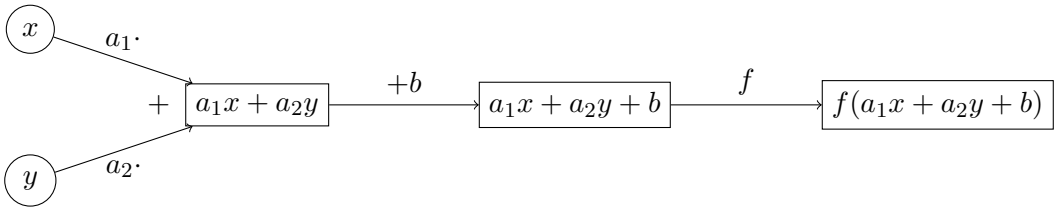


Figure 2: Computation graph of a perceptron.

Since a perceptron only uses one kind of aggregation -the sum-, we shall now only consider computation graphs with one unique operator to aggregate the functions. This operator is denoted + and is implicitly attached to every node in the graph.

In the algorithm 1, we formalize the notion of "function represented by a computation graph" by defining the algorithm to compute this function from the graph. We assume that there is only one node without any outgoing edge, which is the output of the computation graph, noted *out*. We also assume that we have a special function f_v for each input node v. These special functions should be thought of as symbols, such as the "x" in a definition of the form $f(x) = 3x + 2$.

In the section 2.4, we prove that the result does not depend on the topological ordering chosen in the execution of the algorithm.

2.2 Model

In [Green et al., 2007] and [Ramusat, 2022], the authors defined a set of identities and restrictions on the object of their studies (respectively relational databases and graph databases) and then used this set to identify an algebraic structure to theoretically model them.

We follow the same method to characterize the minimal algebraic structure required to model a computation graph. An example of generalized computation graph is given in Figure 3. In what follows, we describe the different properties of computation graphs and traduce them algebraically. The process is summarized in the table of Figure 4 and specific instances where the described properties are necessary are presented in Figure 5. In the examples of Figure 5, the symbolic functions are omitted for better readability.

Algorithm 1 Retrieving a function from a computation graph

Input: Computation Graph $G = (V, E, Fun, Op)$.
Output: The function represented by the graph.

Function Retrieve(G):
  Let T be a topological ordering of (V, E).
  Initialize: $Function[v] =$ None for all $v \in V$
  for each v in T **do**
    if v is an input node **then**
      $Function[v] = f_v$.
    else
      Initialize: $f = 0$
      for each edge $e = (u, v)$ entering v **do**
        $f = f + (Fun(e) \circ Function[u])$
  return $Function[out]$

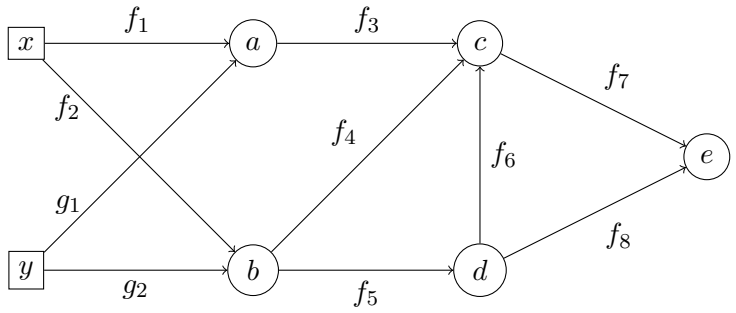


Figure 3: A generalised computation graph.

Structure needed We consider a structure $(F, \circ, +, 0, id)$. The $+$ and $\circ$ are operators $F^2 \to F$ respectively used to model aggregation and composition in the computation graph.

Firstly, since there is no natural order on incoming edges for a node, $+$ must be associative and commutative so the sum on incoming edges is well-defined. For an example, see the Figure 5a.

We require the operator $\circ$ to be associative to ensure modularity. For an example, see the Figure 5b.

To abstract the concept of zero-weight, we require the existence of a neutral element 0 which is a left absorbing element for the $\circ$ operator and which is a neutral element for $+$. For an example, see the Figure 5c.

We require the left distributivity $(f + g) \circ h = f \circ h + g \circ h$ because it is of theoretical interest (it is necessary for the interpretation of near-semirings as sub-near-semirings of the the complete near-semiring over a monoid), because it is a natural identity to interpret the elements as functions and because it allows for a simplification of the computation in some cases. For an example, see the Figure 5d.

Finally, we require the existence of a neutral element id for $\circ$. This might not be crucial, but it has interesting theoretical properties -it matters for theorem 1- and allows some natural representation. For an example, see the Figure 5e.

The axiom identified are those of a near-semiring, with two differences ($+$ is not assumed to be commutative in general and the "id" does not necessarily exist). In our case, we obtain the definition:

Definition 1 (Near-semiring)**.** *A near-semiring $(F, +, \circ, 0_F, id)$ is a set F equiped with two binary operations $+, \circ$ and two distinguished elements $0_F, id$ such that :*

- *$(F, +, 0_F)$ is a commutative monoid;*
- *$(F, \circ, id)$ is a monoid;*

Property on the computation graph	Algebraic translastion of the property
The edges that enter a node are not ordered	$+$ is associative and commutative
The concatenation of two computation graphs is a computation graph that represent the composition of the functions	$\circ$ is associative
There is a notion of zero-weight that model the fact that there is no interaction between two nodes.	There is a 0_F element that is a neutral element for $+$ and that is left absorbing for $\circ$.
We can reuse computation previously done in a natural way.	The operator $\circ$ is right distributive over $+$.
We should be able to model the identity function.	There is a neutral element id for $\circ$.

Figure 4: Motivation of the algebraic structure.

- $\forall (f, g, h) \in F^3$, $(f + g) \circ h = f \circ h + g \circ h$;
- 0_F *is left absorbing for* $\circ$, *i.e. for all* $f \in F$, $0_F \circ f = 0_F$.

Together with this definition comes the notion of morphism of near-semiring and of sub-near-semiring:

A sub-near-semiring of a near-semiring $(F, +, \circ, 0, id)$ is a subset $G \subset F$ such that $0 \in G, id \in G$ and G is stable by $+$ and $\circ$. If G is a sub-near-semiring of $(F, +, \circ, 0, id)$, then $(G, +, \circ, 0, id)$ (for the restriction of operations $+$ and $\circ$ to G) forms a near-semiring.

If $(F, +, \circ, 0, id)$ and $(G, +', \circ', 0', id')$ are two near-semirings, then $\phi : F \to G$ is said to be a near-semiring morphism if it satisfies $\phi(0) = 0', \phi(id) = id', \forall (f, g) \in F^2, \phi(f + g) = \phi(f) +' \phi(g)$ and $\phi(f \circ g) = \phi(f) \circ' \phi(g)$. The image $\phi(F)$ is a sub-near-semiring of G.

2.3 Examples of Near-semirings

Before establishing further theoretical results, we give a few examples of near-semirings.

Near-semiring 1 (Complete near-semiring over a monoid)**.** *Let* $(M, +, 0_M)$ *be a monoid. We define* $\mathcal{F}$ *the set of all functions* $M \to M$. *Then* $(\mathcal{F}, +, \circ, 0_F, id)$ *where* $0_F : x \mapsto 0_M$ *is the zero function and* $id : x \mapsto x$ *is the identity function is a near-semiring, that we will call complete near-semiring over* M. *A particular sub-near-semiring of* $\mathcal{F}$ *is the set of monoid endomorphisms of* M *(it is even a semiring). As we shall see later in this work, this is the most general kind of near-semiring in some sense.*

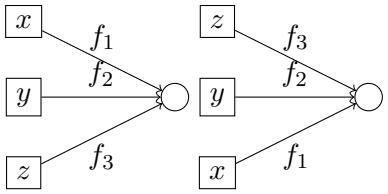
Near-semiring 2. *The* $\mathcal{C}^\infty$ *functions over the real numbers form a near-semiring with usual addition, composition, zero function and identity.*

Near-semiring 3 (Semirings)**.** *Let* $(S, +, \cdot, 0, 1)$ *be a semiring. Then* $(S, +, \cdot, 0, 1)$ *is also a near-semiring. Indeed, the axioms of near-semiring are strictly more general than those of a semiring. The interpretation of semirings as sets of function together with the interpretation of* $\cdot$ *as a composition can be made through the structure of semimodules, which is itself a sub-near-semiring of the complete near-semiring over a monoid.*

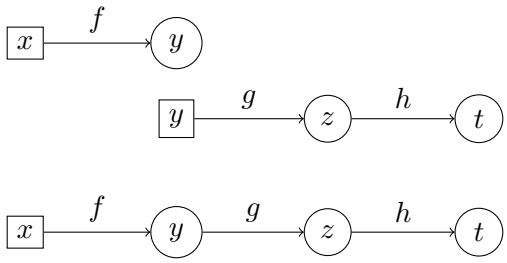
2.4 Properties of Generalized Computation Graphs

We now provide two theoretical properties on computation graphs. These two properties ensure that the model

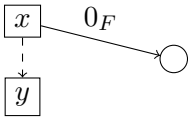
Property 1. *The output of algorithm 1 does not depend on the topological ordering chosen in the execution.*



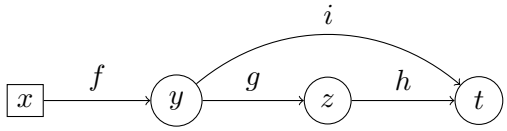
(a) A case that necessitates the "+" operator to be commutative and associative. Indeed, these two graphs are the same represented in two different ways, and the left one represent the element $(f_1 + f_2) + f_3$ whereas the right one represents $(f_3 + f_2) + f_1$. Replacing f_3 by 0 then shows that + must be commutative, and using the commutativity of + shows that the right expression is equal to $f_1 + (f_2 + f_3)$, so the associativity is required too.



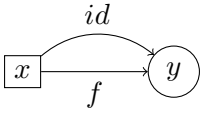
(b) Necessity of the associativity for the modularity. The fact that the graph below, which associated element is $h \circ (g \circ f)$, represents the same element as the composition of the two graphs above, which associated element is $(h \circ g) \circ f$, is equivalent to the associativity of $\circ$. Then we can say without ambiguity that they both represent $h \circ g \circ f$.



(c) Use-cases of the 0 weight. The plain arrow represent an existing edge with weight 0 (in the context of neural network for instance) and the dashed arrow represent an edge that does not exist and could be represented by the 0 element, which could for instance be used to model computation graphs as adjacency matrices.



(d) Illustration of the modularity allowed by the right distributivity. We can factor the expression $i \circ f + h \circ g \circ f$ in the smaller one $(i + g \circ h) \circ f$.



(e) A use case of the identity: representing $f(x) + x$.

Figure 5: The situations that justify the different properties discussed in Figure 4.

Proof. We consider a computation graph $G = (V, E, Fun, Op)$ and two topological orderings T_1, T_2. We note $n = |V|$. We use the notations of algorithm 1 with an index 1 or 2 to refer to the execution that is considered.

We proceed by induction on $i \in [|0, n|]$ with the hypothesis H_i: "For all $1 \leqslant k \leqslant i$, if we note v_k the k-th node according to the ordering T_1, then $Function_1[v_k] = Function_2[v_k]$".

In the base case, $i = 0$ and there is nothing to prove. We now consider $i \in [|0, n|]$, assume H_i is verified and prove that H_{i+1} is verified as well.

We only need to prove that $Function_1[v_{i+1}] = Function_2[v_{i+1}]$.

If v_{i+1} is an input node, then $Function_1[v_{i+1}] = f_{v_{i+1}} = Function_2[v_{i+1}]$.

Else, by definition, $Function_1[v_{i+1}] = \sum_{e=(u,v_{i+1})\in E} Fun(e) \circ Function_1[u]$. However, since all the vertices u that appear in the sum are before v in the topological ordering, by the induction hypothesis this can be rewritten: $Function_1[v_{i+1}] = \sum_{e=(u,v_{i+1})\in E} Fun(e) \circ Function_2[u] = Function_2[v_{i+1}]$, which conclude the proof. □

Note that the only thing required by the proof is that the result of the aggregation operation $+$ (denoted by $\sum$ in the computation) does not depend on the order of its arguments.

Property 2 (Modularity of computation graphs)**.** *We consider two computation graphs G_1, G_2 over the same near-semiring $(F, +, \cdot, 0, id)$. We assume that G_1 has only one output node and that G_2 has only one input node.*

We define $G_{1\circ 2}$ as the computation graph that contains the disjoint union of G_1 and G_2 with one edge with weight id that connects the output of G_1 to the input of G_2. We assume that the symbolic function associated to the input of G_2 is id.

Then we have $Retrieve(G_{1\circ 2}) = Retrieve(G_2) \circ Retrieve(G_1)$.

The assumption done on the symbolic function of the only input of G_2 is natural: the symbolic functions are required to distinguish between the inputs, when there is only one input it is not necessary to use them.

Proof. Let T_1 be a topological ordering of G_1, T_2 be a topological ordering of G_2. Then T which is the concatenation of T_1 and T_2 is a topological ordering of $G_{1\circ 2}$. According to property 1, we can choose any topological ordering for the execution of algorithm 1. Therefore, for $i \in \{1, 2\}$, we consider the execution of algorithm 1 for the topological ordering T_i of G_i and we note F_i the array of functions that is created during this execution.

We now consider an execution of algorithm 1 for the topological ordering T of $G_{1\circ 2}$ and note F the array of functions that is created during the execution. Firstly, it is clear that $\forall v_1 \in V_1, F_1[v_1] = F[v_1]$, and in particular, if out_1 is the output node of G_1, then $Retrieve(G_1) = F_1[out_1] = F[out_1]$. We note $f_1 = F[out_1]$ this value.

We show by induction on the nodes V_2, with the ordering given by T_2, that $F[v_2] = F_2[v_2] \circ f_1$.

The base case is for the input node of G_2, noted in_2. On the one hand, we have $F_2[in_2] = id$ because the symbolic function associated to in_2 is id by hypothesis. On the other hand, $F[in_2] = id \circ F[out_1] = f_1$ because in $G_{1\circ 2}$, in_2 is connected to out_1 by an edge with weight id.

We now assume that we the property holds for all vertices of V_2 that precede a vertex v according to T_2 and we show that the property then holds for v as well.

By definition, $F[v] = \sum_{e=(u,v)\in E_{1\circ 2}} Fun(e) \circ F[u]$. Since v is not the input node of G_2, this can be rewritten: $F[v] = \sum_{e=(u,v)\in E_2} Fun(e) \circ F[u]$. Then, using the induction hypothesis on the u, that

necessarily precede v in the topological ordering, we get:

$$\begin{aligned} F[v] &= \sum_{e=(u,v)\in E_2} Fun(e) \circ F[u] \\ &= \sum_{e=(u,v)\in E_2} Fun(e) \circ (F_2[u] \circ f_1) \\ &= \sum_{e=(u,v)\in E_2} (Fun(e) \circ F_2[u]) \circ f_1 \\ &= (\sum_{e=(u,v)\in E_2} Fun(e) \circ F_2[u]) \circ f_1 \\ &= F_2[v] \circ f_1 \end{aligned}$$

where we used the associativity of $\circ$, the distributivity of $+$ over $\circ$ and the definition of F_2. We use an abuse of notation while referring to Fun as the function that gives the weight of the edges in G_2 and in $G_{1\circ 2}$.

This conclude the proof.

□

Theoretically, this property is interesting because it shows that the two conditions that were necessary for modularity -distributivity and associativity of $\circ$- are sufficient.

It also has practical influence because it means that when we have computed the function associated to a sub-graph, then we can reuse it in different settings, which enable the use of techniques like dynamic programming.

2.5 Universal Object

In this section we identify the sub-near-semiring generated by a subset $G \subset F$ of a near-semiring F. This notion matters because this provides the form of the result that we can expect from the algorithm *Retrieve*. For instance, in the context of databases, the universal object for semiring provenance is the semiring of polynomials over integers $\mathbb{N}[X]$ [Green et al., 2007]. Similarly, in [Ramusat, 2022], the provenance over a graph database between two points x and y could be expressed as the sum of the weight of the paths between two points, which is also a polynomial on the weights of the edges.

In our settings, unfortunately, the universal object is slightly more complicated, as shown below.

Formally, given a near-semiring F, we want to characterize the sub-near-semiring generated by a subset $G \subset F$. This notion makes sense for the usual reason: an intersection of sub-near-semiring is a sub-near-semiring itself, and we note $< G >$ this sub-near-semiring .

For this purpose we define a sequence of sets (G_n) by $G_0 = \{0, id\} \cup G$ and

$$G_{n+1} = \left\{ g \circ \left(\sum_{i=1}^{k} g_i \right) \middle| \; k \in \mathbb{N}, g \in G, (g_i)_{1\leqslant i\leqslant n} \in (G_n)^k \right\}.$$

We can now state the property:

Property 3. $< G >= \underset{n\in\mathbb{N}}{\cup} G_n$.

Indeed, $G \subset G_0 \subset \underset{n\in\mathbb{N}}{\cup} G_n$, then we show by induction that $\forall n \in \mathbb{N}, G_n \subset < G >$ and finally we show that $\underset{n\in\mathbb{N}}{\cup} G_n$ is indeed a sub-near-semiring of F.

For instance, the result of *Retrieve* on the computation graph of Figure 3 is

$$f_7 \circ (f_3 \circ (f_1 \circ x + g_1 \circ y) + f_4 \circ (f_2 \circ x + g_2 \circ y)) + f_8 \circ f_4 \circ (f_2 \circ x + g_2 \circ y).$$

This expression, that is already complicated for a small graph, cannot be expressed in much simpler way due to the result of property 3.

2.6 Generality of the Complete Near-semiring over a Monoid.

The generality of the near-semiring structure is needed to model computation graphs as shown earlier, but to instantiate the theory efficiently we need to understand how to create near-semirings. The theorem shown in this section provide such a tool, by giving a form for near-semirings.

Theorem 1. *Universal Form of Near-semirings*
It is equivalent to be given:

1. *a near-semiring* $(F, +, \circ, 0, id)$
2. *a commutative monoid* $(M, +, 0)$ *together with a set of functions* $M \to M$ *containing* 0 *and* id *and stable by* $\circ$ *and* $+$*. (I.e. a sub-near-semiring of the complete near-semiring over* M*.)*

Proof. Firstly, we assume that we are given a monoid $(M, +, 0)$ and a set of functions $M \to M$ containing 0, id and stable by $+$ and $\circ$ like in two. This precisely means that we are given a sub-near-semiring of the complete near-semiring over $(M, +, 0)$, and hence a near-semiring.

Secondly, if we are given a near-semiring $(F, +, \circ, 0, id)$, we define for an element f the function

$$\bar{f} : \begin{cases} F & \to & F \\ g & \mapsto & f \circ g \end{cases},$$

then we define the function $\phi : \begin{cases} F & \to & ((F,+,0) \to (F,+,0)) \\ f & \mapsto & \bar{f} \end{cases}$.

The function ϕ is a morphism of near-semirings. Indeed:

- $\phi(0)$ is the zero function since zero is left absorbing,
- $\phi(id)$ is the identity function because $\forall g \in F, id \circ g = g$,
- $\forall f_1, f_2 \in F^2,\ \forall g \in F,\ \phi(f_1 + f_2)(g) = (f_1 + f_2) \circ g = f_1 \circ g + f_2 \circ g = \phi(f_1)(g) + \phi(f_2)(g)$, hence $\phi(f_1 + f_2) = \phi(f_1) + \phi(f_2)$
- $\forall f_1, f_2 \in F^2,\ \forall g \in F,\ \phi(f_1 \circ f_2)(g) = (f_1 \circ f_2) \circ g = f_1 \circ (f_2 \circ g) = \phi(f_1)(f_2 \circ g) = (\phi(f_1) \circ \phi(f_2))(g)$, hence $\phi(f_1 \circ f_2) = \phi(f_1) \circ \phi(f_2)$

Therefore, $\phi(F)$ is a sub-near-semiring of the complete near-semiring over the monoid $(F, +, 0)$.

□

3 Instantiation of the Theory

3.1 Layer-Wise Relevance Propagation

Layer-Wise Relevance Propagation (LRP) is a technique used to explain the prediction made by a neural network on one of its execution [Montavon et al., 2019]. The idea of the technique is to propagate backwards the contribution (or the *relevance*) of neurons in the network to the final prediction of the model. The general formula is

$$R_j = \sum_k \frac{z_{j,k}}{\sum_j z_{j,k}} R_k.$$

The value R_j is the score of the neuron j, and it is computed by summing over all neurons k in the next layer the term $\frac{z_{j,k}}{\sum_j z_{j,k}} R_k$, where R_k is the relevance of neuron k and $\frac{z_{j,k}}{\sum_j z_{j,k}}$ represents the extent to which neuron j contributed to the relevance of the neuron k.

The normalization term ensures that vanishing phenomenons cannot occur: the sum of the relevances of the neurons on a given layer is preserved.

We should now discuss the interpretation of LRP as an instantiation of our model.

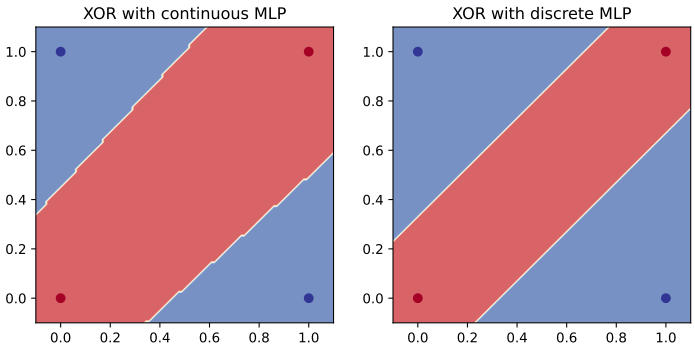


Figure 6: The decision boundaries of the network trained to learn *xor* before and after quantization. The weights are transformed from float to integers.

We can model LRP with generalized computation graphs. Indeed, the input nodes of the computation graphs are the output neurons of the network (or even the only neuron corresponding to the class predicted, since the value of other neurons is set to zero), the edges of the computation graph are the reversed edges of the neuron and the associated function is the multiplication by the scalar $\frac{z_{j,k}}{\sum_j z_{j,k}}$ (between neurons k and j).

However, since the computations made to compute the relevance depend on an execution, it might be of limited interest to construct the computation graph to use it only one time.

3.2 Quantization

The result of theorem 1 tells that we can execute neural networks on monoids, and not only on real numbers as we usually do.

This method actually already exists and is called quantization [**?**]. The method consists of training neural networks on high precision representation of real numbers and then discretize the weights of the network. This allows for faster execution of the neural networks, that uses less memory and bandwidth.

I have done an experiment on a simple example of a network trained to learn the *xor* function, and the result suggest that the method leads to simpler model, that may be less precise but could also be more reliable and interpretable -at least for small ones. The experiment are shown in Figure 6.

4 Conclusion

[TODO]

Computation Graphs Bibliography

[CompGreen et al., 2007] Green, T. J., Karvounarakis, G., and Tannen, V. (2007). Provenance semirings. In *Proceedings of the twenty-sixth ACM SIGMOD-SIGACT-SIGART symposium on Principles of database systems*, pages 31–40, Beijing China. ACM.

[CompMontavon et al., 2019] Montavon, G., Binder, A., Lapuschkin, S., Samek, W., and Müller, K.-R. (2019). Layer-Wise Relevance Propagation: An Overview. In Samek, W., Montavon, G., Vedaldi, A., Hansen, L. K., and Müller, K.-R., editors, *Explainable AI: Interpreting, Explaining and Visualizing Deep Learning*, volume 11700, pages 193–209. Springer International Publishing, Cham. Series Title: Lecture Notes in Computer Science.

[CompRamusat, 2022] Ramusat, Y. (2022). *The semiring-based provenance framework for graph databases*. phdthesis, Université Paris sciences et lettres.

[CompWang and Zhao, 2023] Wang, L. and Zhao, J. (2023). *Computation Graph*, pages 149–189. Apress, Berkeley, CA.

5 Extra work - GNN Stability

While investigating the theoretical modeling of neural network, I met a Ph.D student that was researching the application of the graph neural network (GNN) framework for databases.

GNNs are a class of neural network that is meant to represent graph-structured data in $\mathbb{R}^d$ while taking into account the relations between the data points and initial feature information on the nodes. Such representations, or embeddings, are valuable because we can then apply usual machine learning techniques to the transformed data. However, for the method to be effective on perturbed databases, we need to ensure that the embeddings of the perturbed database are close the embeddings of the original database. This notion is referred to as stability.

My contribution in this work was to adapt result on stability to our precise setting. The more restrictive hypotheses used in our work even allowed me to improve existing results.

5.1 Definition of GNNs

We begin by defining the GNNs that we use in this work and describe how we can embed nodes using this method. Further theory on GNNs can be found in [**?**].

Definition 2 (GNNs)**.** *A graph neural network for graphs with n nodes is a function* $\Phi : S_n(\mathbb{R}) \times R^n \to \mathbb{R}^n$.

5.2 Formal Framework for Stability

To measure the distance between two graph shift operators, and consequently the distance between the graphs they are derived from, we use $d_{\mathcal{P}}(S, \hat{S})$, noted $||S - \hat{S}||_{\mathcal{P}}$ in [Gama et al., 2020], defined as $d_{\mathcal{P}}(S, \hat{S}) = \min_{P \in \mathcal{P}} ||S - P\hat{S}P^T||$ where $\mathcal{P}$ is the set of permutation matrices. We change the notations to highlight the fact that the quantity depends on the two matrices $S, \hat{S}$ and not on the difference $S - \hat{S}$. The definition of $d_{\mathcal{P}}$ can be extended to general continuous operators $\Psi, \hat{\Psi} : \mathbb{R}^N \to \mathbb{R}^N$ by $d_{\mathcal{P}}(\Psi, \hat{\Psi}) = \min_{P \in \mathcal{P}} \max_{||x||=1} ||P^T\Psi(x) - \hat{\Psi}(P^T x)||$.

Limitations There are two main challenges to apply the preceding framework. Firstly, computing $d_{\mathcal{P}}(S, \hat{S})$ is more general than determining if the graphs are isomorphic, so it is not feasible for large n in general. (Indeed, if S is the adjacency matrix, then two graphs G and $\hat{G}$ are isomorphic if and only if there exists $P \in \mathcal{P}$ s.t. $S = P\hat{S}P^T$, which is equivalent to $d_{\mathcal{P}}(S, \hat{S}) = 0$.) Secondly, we can only compare matrices that have the same size, i.e. graphs that have the same number of nodes. However, we seek to measure the perturbation induced by the deletion of tuples in the database, which corresponds to node deletion in the graph.

Solution used in this work We consider a database D with associated graph G. Let T be a set of tuples of D, let $\hat{D}$ be the database D without the tuples in T and let $\hat{G}$ be its associated graph. We define their two graph shift operators S and $\hat{S}$. There are two equivalent points of view for our approach:

- We fill the matrix $\hat{S}$ with rows and columns of 0s so its shape matches the shape of S. Then we consider the permutation σ_0 that matches the remaining nodes in $\hat{G}$ with their original node in G and matches the rows/columns of 0s with the nodes in G that disappeared in $\hat{G}$. The permutation σ_0 provides us a permutation matrix P_0 and we bound $d_{\mathcal{P}}(S, \hat{S})$ by $||S - P_0\hat{S}P_0^T||_{op}$.
- We do not delete the nodes we are supposed to delete, but delete their edges instead. This yields a graph $\hat{G}'$ with exactly the same nodes as G but some missing edges, and we compute $||S - \hat{S}'||_{op}$.

5.3 Theoretical results

We take advantage of the fact that we only use filters that are polynomial of order 1 to refine the theorem 4 of [Gama et al., 2020]. The two main improvements that are allowed by this simplification is the fact that the inequality is now a global inequality and there is no dependency in N.

Theorem 2. *Let $\Phi(\cdot,\cdot)$ be a GNN with L layers, less than F features per layer and that only uses filters of the form $H(X) = aX + b$. We assume that the non-linearities σ in Φ are 1-Lipschitz and satisfy $\sigma(0) = 0$. Let $S, \hat{S} \in \mathbb{R}^{N\times N}$ be two symmetric matrices. We note $||H||_\infty = \max_{H\in\Phi,\ \lambda\in\sigma(S)\cup\sigma(\hat{S})} |H(\lambda)|$ the maximum of the value $|H(\lambda)|$ over all filters H that appear in Φ and all λ that are eigenvalues of S or $\hat{S}$ and we note $A = \max_{H(X)=aX+b\in\Phi} |a|$.*

Then, for all $x \in \mathbb{R}^N$, we have:

$$||\Phi(S,x) - \Phi(\hat{S},x)|| \leqslant LA(F||H||_\infty)^{L-1}||S-\hat{S}||_{op}||x||.$$

There are a few remarks to be done about the theorem. Firstly, the proof provides a more specific bound: we can replace $LA(F||H||_\infty)^{L-1}$ by $B_L = \left(\prod_{i=1}^{L-1} F_i\right)\cdot\sum_{i=1}^{L}\left[\left(\prod_{j=L-i+1}^{L-1}||H^{(i)}||_\infty\right)\cdot A^{(L-i)}\cdot\left(\prod_{j=0}^{L-i-1}||H^{(i)}||_\infty\right)\right]$ where F_i is the number of features at the i-th layer, $||H^{(i)}||_\infty$ is the maximum of all values $|H^{(i)}(\lambda)|$ for λ ranging over the eigenvalues of S and $\hat{S}$ and $H^{(i)}$ ranging over the filters between the i-th and the $i+1$-th layer and $A^{(i)}$ is the maximum of the coefficient $|a|$ for all filers taps between the i-th and the $i+1$-th layer that can be written $H(X) = aX + b$.

This bound is much less readable, but it allows to take into account irregularities between layers. This can make a big difference when the number of layers grows and there is only one layer with a big amount of features or there is only one layer with a big value of $A^{(i)}$.

Secondly, the theorem is wrote for a general couple of matrices $(S, \hat{S})$ but we can instantiate it with the $d_{\mathcal{P}}$ distance:

Corollary 2.1. Given a GNN Φ satisfying the hypotheses of the theorem 2, the following equality holds:

$$d_{\mathcal{P}}(\Phi(S,\cdot),\Phi(\hat{S},\cdot)) \leqslant LA(F||H||_\infty)^{L-1}d_{\mathcal{P}}(S,\hat{S}).$$

Proof. Firstly, we show how to deduce the corollary from the theorem. We consider $P_0 \in \mathcal{P}$ such that $d_{\mathcal{P}}(S,\hat{S}) = ||S - P_0\hat{S}P_0^T||_{op}$. The theorem then provides the inequality, for $||x|| = 1$,

$$\begin{aligned}||\Phi(S,x) - \Phi(P_0\hat{S}P_0^T,x)|| &\leqslant LA(F||H||_\infty)^{L-1}||S - P_0\hat{S}P_0^T||_{op}\\ &= LA(F||H||_\infty)^{L-1}d_{\mathcal{P}}(S,\hat{S})\end{aligned}$$

and since

$$\begin{aligned}d_{\mathcal{P}}(\Phi(S,\cdot),\Phi(\hat{S},\cdot)) &= \min_{P\in\mathcal{P}}\max_{||x||=1}||P^T\Phi(S,x) - \Phi(\hat{S},P^Tx)||\\ &= \min_{P\in\mathcal{P}}\max_{||x||=1}||\Phi(S,x) - P\Phi(\hat{S},P^Tx)||\\ &= \min_{P\in\mathcal{P}}\max_{||x||=1}||\Phi(S,x) - \Phi(P\hat{S}P^T,x)||\\ &\leqslant \max_{||x||=1}||\Phi(S,x) - \Phi(P_0\hat{S}P_0^T,x)||,\end{aligned}$$

then we have for the x that reaches the max:

$$\begin{aligned}d_{\mathcal{P}}(\Phi(S,\cdot),\Phi(\hat{S},\cdot)) &\leqslant ||\Phi(S,x) - \Phi(P\hat{S}P^T,x)||\\ &\leqslant LA(F||H||_\infty)^{L-1}d_{\mathcal{P}}(S,\hat{S}).\end{aligned}$$

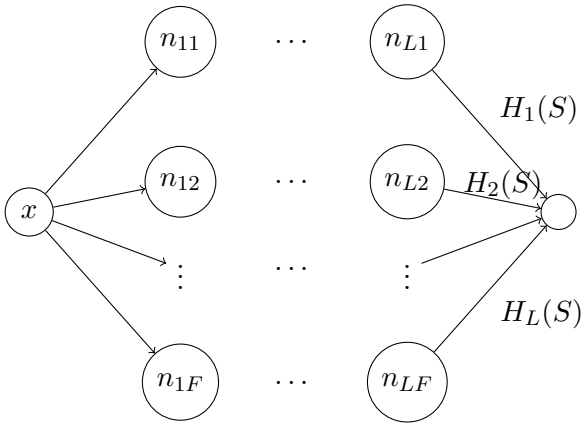


Figure 7: Shape of Φ.

We now prove the theorem 2. The method used is very close from what is done in [Gama et al., 2020]. We show a more precise theorem by using the bound

$$B_L = \left(\prod_{i=1}^{L-1} F_i\right) \cdot \sum_{i=1}^{L} \left[\left(\prod_{j=L-i+1}^{L-1} ||H^{(i)}||_\infty\right) \cdot A^{(L-i)} \cdot \left(\prod_{j=0}^{L-i-1} ||H^{(i)}||_\infty\right) \right]$$

rather than $LA(F||H||_\infty)^{L-1}$. We check that $B_L \leqslant LA(F||H||_\infty)^{L-1}$ by bounding all the coefficient that depends on a layer by their global counterpart ($A^{(L-i)} \leqslant A$, $F_i \leqslant F$ and $||H^{(i)}||_\infty \leqslant ||H||_\infty$).

We begin with a lemma:

Lemma 3. We consider a GNN Φ satisfying the hypotheses of 2, S a symmetric matrix and x a vector. Then we have:

$$||\Phi(S,x)|| \leqslant \left(\prod_{i=0}^{L-1} F_i\right) \left(\prod_{i=0}^{L-1} ||H^{(i)}||_\infty\right) ||x||$$

Indeed, we show this lemma by induction on the number of layers of Φ. For a GNN Φ with only one layer, since the input and output layers can only contain one feature, then Φ is of the form $\Phi(S,x) = \sigma(H(S)x)$. Consequently,

$$\begin{aligned} ||\Phi(S,x)|| &\leqslant ||H(S)x|| \\ &\leqslant ||H^{(0)}||_\infty ||x|| \end{aligned}$$

where we used $||H(S)||_{op} \leqslant ||H^{(0)}||$ which directly follows from the definition of $||H^{(0)}||$. This proves that the lemma holds for the initial case.

We now consider $L \in \mathbb{N}^*$ and we assume that the lemma is true for all GNNs with L layers satisfying the hypotheses.

Let $\Phi(\cdot,\cdot)$ be a GNN with $L+1$ layers satisfying the hypotheses, let S be a symmetric matrix and let x be a vector.

By definition of the GNNs in this work, Φ has the form shown in figure 7. We define the function $\Phi_i^{(L)}(S,x)$ that outputs the vector contained in the neuron n_{Li} (the i-th neuron of the L-th layer, see figure 7) during the execution of Φ. The function $\Phi_i^{(L)}$ is a GNN itself, with only L layers.

By definition of Φ, we can then write:

$$\Phi(S,x) = \sigma\left(\sum_{i=1}^{F_L} H_i(S)\Phi_i^{(L)}(S,x)\right).$$

As a consequence we have the inequalities:

$$\begin{aligned}
||\Phi(S,x)|| &\leqslant \sum_{i=1}^{F_L} ||H_i(S)\Phi_i^{(L)}(S,x)|| \\
&\leqslant F_L ||H^{(L)}||_\infty ||\Phi_i^{(L)}(S,x)|| \\
&\leqslant F_L ||H^{(L)}||_\infty \left(\prod_{i=0}^{L-1} F_i\right) \left(\prod_{i=0}^{L-1} ||H^{(i)}||_\infty\right) ||x|| \\
&= \left(\prod_{i=0}^{L} F_i\right) \left(\prod_{i=0}^{L} ||H^{(i)}||_\infty\right) ||x||
\end{aligned}$$

where we used the induction hypothesis to bound $||\Phi_i^{(L)}(S,x)||$. This concludes the proof of the lemma.

We now prove theorem 2 by induction on the number of layers L as well. Firstly, if we consider a GNN with 1 layer, then $\Phi(S,x)$ is $\sigma(H(S)x)$ with $H(S) = aS + bI_N$. Given two symmetric matrices S and $\hat{S}$ and a vector $x \in \mathbb{R}^N$, the theorem is written: $||\sigma(H(S)x) - \sigma(H(\hat{S})x)|| \leqslant B_1 ||S - \hat{S}||_{op} ||x||$ with $B_1 = A^{(1)} = |a|$.

This holds since:

$$\begin{aligned}
||\sigma(H(S)x) - \sigma(H(\hat{S})x)|| &\leqslant ||H(S)x - H(\hat{S})x|| \\
&= ||a(S - \hat{S})x|| \\
&\leqslant |a| ||S - \hat{S}||_{op} ||x||.
\end{aligned}$$

We now consider $L \in \mathbb{N}^*$ and we assume that the theorem is true for all GNNs with L layers satisfying the hypotheses. I.e., if Ψ is such a GNN, $||\Psi(S,x) - \Psi(\hat{S},x)|| \leqslant B_L ||S - \hat{S}||_{op} ||x||$.

We consider a GNN Φ with $L+1$ layers and use the exact same notations as in the proof of the lemma.

We begin by bounding $\Phi(S,x) - \Phi(\hat{S},x)$ with the $\Phi_i^{(L)}$:

$$\begin{aligned}
||\Phi(S,x) - \Phi(\hat{S},x)|| &= ||\sum_{i=1}^{F_L} H_i(S)\sigma(\Phi_i^{(L)}(S,x)) - H_i(\hat{S})\sigma(\Phi_i^{(L)}(\hat{S},x)) \,|| \\
&\leqslant \sum_{i=1}^{F_L} ||H_i(S)\sigma(\Phi_i^{(L)}(S,x)) - H_i(\hat{S})\sigma(\Phi_i^{(L)}(\hat{S},x)) \,|| \\
&\leqslant \sum_{i=1}^{F_L} ||H_i(S) \left(\sigma(\Phi_i^{(L)}(S,x)) - \sigma(\Phi_i^{(L)}(\hat{S},x))\right) || \\
&+ \sum_{i=1}^{F_L} || \,(H_i(S) - H_i(\hat{S}))\sigma(\Phi_i^{(L)}(\hat{S},x)) \,|| \qquad (1)
\end{aligned}$$

We should now bound both terms separately. We begin with $||H_i(S) \left(\sigma(\Phi_i^{(L)}(S,x)) - \sigma(\Phi_i^{(L)}(\hat{S},x))\right) ||$. Using the definition of $||H^{(L)}||_\infty$ and the induction hypothesis, we get:

$$\begin{aligned}
&||H_i(S) \left(\sigma(\Phi_i^{(L)}(S,x)) - \sigma(\Phi_i^{(L)}(\hat{S},x))\right) || \qquad (2) \\
&\leqslant ||H^{(L)}||_\infty ||\sigma(\Phi_i^{(L)}(S,x)) - \sigma(\Phi_i^{(L)}(\hat{S},x))|| \\
&\leqslant ||H^{(L)}||_\infty ||\Phi_i^{(L)}(S,x) - \Phi_i^{(L)}(\hat{S},x)|| \\
&\leqslant ||H^{(L)}||_\infty B_L ||S - \hat{S}||_{op} ||x||. \qquad (3)
\end{aligned}$$

For the second term, using the definition of $A^{(L)}$ and the lemma, we get:

$$\begin{aligned}
&||(H_i(S) - H_i(\hat{S}))\sigma(\Phi_i^{(L)}(\hat{S}, x))|| \\
&\qquad \leqslant ||H_i(S) - H_i(\hat{S})||_{op}||\sigma(\Phi_i^{(L)}(\hat{S}, x))|| \\
&\qquad \leqslant A^{(L)}||S - \hat{S}||_{op}||\Phi_i^{(L)}(\hat{S}, x)|| \\
&\qquad \leqslant A^{(L)}||S - \hat{S}||_{op}\left(\prod_{i=0}^{L-1} F_i\right)\left(\prod_{i=0}^{L-1}||H^{(i)}||_\infty\right)||x||. \qquad (4)
\end{aligned}$$

Combining the bounds given by inequalities 3 and 4 in the inequality 1 yields

$$\begin{aligned}
||\Phi(S, x) - \Phi(\hat{S}, x)|| &\leqslant \sum_{i=1}^{F_L}||H^{(L)}||_\infty B_L||S - \hat{S}||_{op}||x|| \\
&\quad + \sum_{i=1}^{F_L} A^{(L)}\left(\prod_{i=0}^{L-1} F_i\right)\left(\prod_{i=0}^{L-1}||H^{(i)}||_\infty\right)||S - \hat{S}||_{op}||x|| \qquad (5) \\
&\leqslant \left(F_L||H^{(L)}||_\infty B_L + F_L A^{(L)}\left(\prod_{i=0}^{L-1} F_i\right)\left(\prod_{i=0}^{L-1}||H^{(i)}||_\infty\right)\right)||S - \hat{S}||_{op}||x||. \qquad (6)
\end{aligned}$$

Given that $F_L||H^{(L)}||_\infty B_L + F_L A^{(L)}\left(\prod_{i=0}^{L-1} F_i\right)\left(\prod_{i=0}^{L-1}||H^{(i)}||_\infty\right) = B_{L+1}$, this can be rewritten:

$$||\Phi(S, x) - \Phi(\hat{S}, x)|| \leqslant B_{L+1}||S - \hat{S}||_{op}||x||, \qquad (7)$$

which shows that the theorem holds for GNN with $L + 1$ layers and concludes the proof.

□

5.4 Node embedding stability

In this section, we discuss two corollaries of the theorem 2 that translate the original result in two stability properties at the node embedding level. Like for the theorem, in the bounds we can replace $LA(F||H||_\infty)^{L-1}$ by B_L.

The node embeddings are defined in section **??**.

Corollary 3.1. We consider a GNN Φ satisfying the hypotheses of theorem 2, and a couple of graph $G, \hat{S}$ with their associated shift operators $S, \hat{S}$. We assume that all the columns of the initialisation matrices $X^{(0)}$ are normalized. If we consider the i-th nodes of G and $\hat{G}$, noted v_i and v_i' and assume that their k-hop are equal, then we have the following property:

$$\begin{aligned}
&||\Phi(S, X^{(0)})_{v_i} - \Phi(\hat{S}, X^{(0)}_{v_i'}|| \\
&\qquad \leqslant \sqrt{d}B_L^{(k)}||S - \hat{S}||_{op} \qquad (8)
\end{aligned}$$

where we define

$$B_L^{(k)} = \left(\prod_{i=1}^{L-1} F_i\right) \cdot \sum_{i=k+1}^{L}\left[\left(\prod_{j=L-i+1}^{L-1}||H^{(i)}||_\infty\right) \cdot A^{(L-i)} \cdot \left(\prod_{j=0}^{L-i-1}||H^{(i)}||_\infty\right)\right].$$

We can bound $B_L^{(k)}$ is 0 if $L \geq k$ and it can be bounded by $(L - k)A(F||H||_\infty)^{L-1}$ otherwise.

The hypothesis of normalization is not necessary, it is there so the statement is more readable. Noting C_i the columns of X, we could remove the hypothesis and replace $\sqrt{d}$ by $\sqrt{\sum_{i=1}^{d}||C_i||^2}$.

Corollary 3.2. We consider a GNN Φ satisfying the hypotheses of theorem 2, and a couple of graph $G, \hat{S}$ with their associated shift operators $S, \hat{S}$. We assume that all the columns of the initialisation matrices $X^{(0)}$ are normalized. We can control the total squared distances between the embeddings:

$$\sum_{i=1}^{N} ||\Phi(S, X^{(0)})_{v_i} - \Phi(\hat{S}, X^{(0)})_{v_i'}||^2 \leqslant dM^2 \tag{9}$$

where M is a bound of theorem 2, i.e. $M = LA(F||H||_\infty)^{L-1}||S - \hat{S}||_{op}$ or $M = B_L||S - \hat{S}||_{op}$.

This last property is interesting because it ensures that for most nodes $||\Phi(S, X^{(0)})_{v_i} - \Phi(\hat{S}, X^{(0)})_{v_i'}||^2 \leqslant \frac{\sqrt{d}M}{\sqrt{N}}$. Since the bound dM^2 does not depend on N, this means that using a GNN with fixed parameters on large database gives reliable embeddings for the majority.

The worst case distance for two embeddings can still be relatively large, it is bounded by

$$\begin{aligned} ||\Phi(S, X^{(0)})_{v_i} - \Phi(\hat{S}, &X^{(0)})_{v_i'}|| \\ &\leqslant \sqrt{\sum_{i=1}^{N} ||\Phi(S, X^{(0)})_{v_i} - \Phi(\hat{S}, X^{(0)})_{v_i'}||^2} \\ &\leqslant \sqrt{d}M, \end{aligned}$$

but this cannot happen for several nodes at the same time.

Proof. We prove the corollary 3.2. We consider Φ, S, $\hat{S}$ and $X^{(0)}$ as in the statement of the corollary.

By definition of the embedding, $||\Phi(S, X^{(0)})_{v_i} - \Phi(\hat{S}, X^{(0)})_{v_i'}|| = ||L_i||^2$ where L_i is the i-th line of the matrix $\Phi(S, X^{(0)}) - \Phi(\hat{S}, X^{(0)})$. Therefore,

$$\begin{aligned} \sum_{i=1}^{N} ||\Phi(S, X^{(0)})_{v_i} - \Phi(\hat{S}, X^{(0)})_{v_i'}||^2 &= \sum_{i=1}^{N} ||L_i||^2 \\ &= \sum_{j=1}^{d} ||C_j||^2 \\ &= \sum_{j=1}^{d} ||\Phi(S, C_j^{(0)}) - \Phi(\hat{S}, C_j^{(0)})||^2 \end{aligned}$$

where C_j is the j-th column of the matrix $\Phi(S, X^{(0)}) - \Phi(\hat{S}, X^{(0)})$ and $C_j^{(0)}$ is the j-th column of $X^{(0)}$.

Since theorem 2 ensures that $||\Phi(S, C_j^{(0)}) - \Phi(\hat{S}, C_j^{(0)})|| \leqslant M$, we deduce:

$$\sum_{i=1}^{N} ||\Phi(S, X^{(0)})_{v_i} - \Phi(\hat{S}, X^{(0)})_{v_i'}||^2 \leqslant dM^2.$$

□

GNN Bibliography

[GnnGama et al., 2020] Gama, F., Bruna, J., and Ribeiro, A. (2020). Stability properties of graph neural networks. *IEEE Transactions on Signal Processing*, 68:5680–5695.