Evaluating Transformers Learning by Representing Self-Attention Weights as a Graph

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Keywords: Explainability, Graph Visualization, Self-Attention, Health Data.

Abstract: Transformers architectures have established themselves as the state of the art for sequential data processing, with applications ranging from machine translation to the processing of Electronic Health Records (EHR). These complex data present a particular challenge in terms of explainability, which is a crucial aspect for their adoption in the healthcare field, subject to strict ethical and legal requirements. To address this challenge, we propose an approach to represent learning through graphs by exposing the self-attention links between tokens. We introduce a metric to assess the relevance of the connections learned by the model, in comparison with medical expertise. We apply our approach to the Behrt model, designed to predict future hospital visits based on sequences of previous visits, trained on data from the French National Health Data System. Our experiments show that our method facilitates understanding of model learning, and enables a better appreciation of the influence of diagnoses on each other, as well as of the biases present in the data, than global model evaluation measures.

1 INTRODUCTION

Since their introduction (Vaswani et al., 2017), Transformers architectures (Lin et al., 2022) have been recognized as the state of the art for processing sequential data (Wen et al., 2023), primarily due to their self-attention mechanism. This mechanism effectively captures the relationships between different elements (tokens) of a sequence while minimizing the vanishing gradient problem (Bengio et al., 1994) often encountered with recurrent architectures. Some of the best-known models using this technology include BERT (Bidirectional Encoder Representations from Transformers) (Devlin et al., 2019), GPT (Generative Pre-trained Transformer) (Radford et al., 2018), and T5 (Raffel et al., 2020), which have revolutionized the field of natural language processing.

Initially introduced for machine translation task (Vaswani et al., 2017), Transformers are now commonly used to process all forms of sequential data, including Electronic Health Records (EHR) (Nerella et al., 2023). EHR contains a multitude of complex data. This includes ICD (International Classification of Diseases)[1] codes for diagnoses and medications, as well as demographic information and treatment histories, which are recorded at each patient visit. The complexity of these data stems not only from their volume and diversity, but also from their structuring into temporal sequences, which capture cycles of diagnosis, treatment and patient follow-up, including potential re-admissions.

Although the adaptation of natural language processing methods for EHR data is very promising, the lack of explainability raises legal and ethical issues that constitute a significant obstacle on the deployment of these methods for decision support in the healthcare field (Amann et al., 2020; Shortliffe et al., 2018). It is currently possible to explain model learning by visualizing learned self-attention weights, but this is done on a few examples, often to show what the model has learned well, without comparison with a ground truth (Siebra et al., 2024).

To address this problem, we propose an approach for understanding and validating the learning of a model based on self-attention mechanisms. This framework consists in representing, in the form of graphs, the links between input tokens, weighted by the self-attention weights learned by the model. Each

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[1] The International Classification of Diseases is a medical classification used worldwide for epidemiological, health management and clinical purposes.

Leygonie, R., Lobry, S. and Wendling, L.
Evaluating Transformers Learning by Representing Self-Attention Weights as a Graph.
DOI: 10.5220/0013111400003912
Paper published under CC license (CC BY-NC-ND 4.0)
In *Proceedings of the 20th International Joint Conference on Computer Vision, Imaging and Computer Graphics Theory and Applications (VISIGRAPP 2025) - Volume 1: GRAPP, HUCAPP and IVAPP*, pages 695-705
ISBN: 978-989-758-728-3; ISSN: 2184-4321
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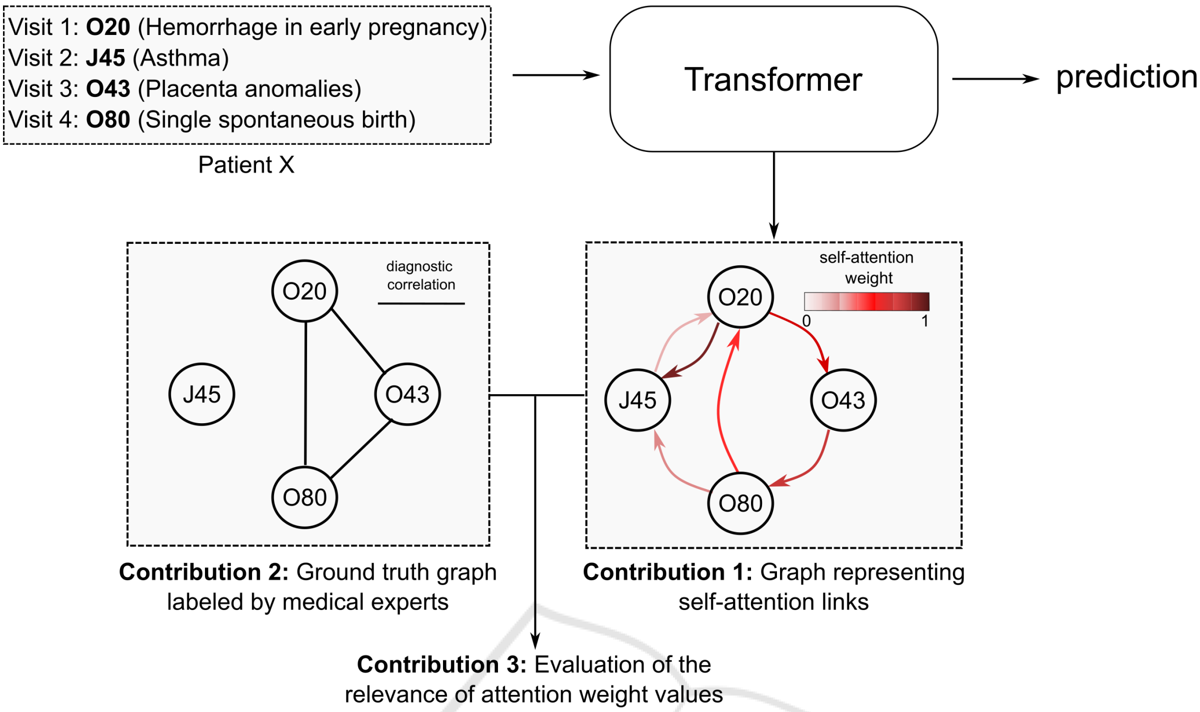


Figure 1: Overview of the proposed approach. Given a sequence of diagnostics input into a Transformer model, we extract the self-attention weights learned by the model between each pair of tokens and represent them as a graph, where each node is a diagnostic and each directed edge from node A to node B represents the self-attention weight node A gives to node B during the model's prediction. We evaluate this graph against a graph representing medical expertise to assess the relevance of the self-attention weights learned by the model.

link in the graph thus represents the relative importance of each token in relation to the others, in a precise data sample. We then evaluate the graph against a ground truth collected from experts to obtain a relevance score for the self-attention links learned by the model. Figure 1 illustrates the proposed approach.

To assess our methodology we apply this approach to a specific model, Behrt (Li et al., 2020), which has been trained on data from the French National Health Data System (SNDS). This model aims at predicting the next hospital visit of a patient given a sequence of previous visits. We apply our approach on two different use cases, illustrating the versatility and effectiveness of our method. The results show that our method can be used to understand and validate model learning. In addition, the use of graphical representations helps users to understand more directly the connections that the model has learned, which is crucial for increasing the confidence of healthcare professionals in using the model's predictions in concrete clinical situations. In this work, we introduce four contributions:

- **Contribution 1.** We propose a method that graphically represents the interactions between tokens learned by the model.
- **Contribution 2.** We propose an approach for modeling medical expertise as a graph.
- **Contribution 3.** We introduce a new metric to evaluate the relevance of the connections learned by the model by comparing them to medical expertise.
- **Contribution 4.** We validate our method through two use cases.

The paper is structured as follows. In Section 2, we review existing works on adapting Transformers to electronic health record (EHR) data, as well as the explainability methods used to validate these models. Section 3 details our proposed methodology. Experimental protocols are explained in Section 4, while the results obtained are presented in Section 5 and discussed in Section 6.

2 RELATED WORK

2.1 Transformers for Health Data

For several years, researchers have propose to exploit data from the International Classification of Diseases

(ICD), notably for the task of predicting future diagnoses (Nerella et al., 2023). Behrt (Li et al., 2020), an adaptation of BERT for EHR data, is pre-trained using a masked language model before being trained on sequences of ICD codes and age data to predict future diagnoses. Hi-BEHRT (Li et al., 2022), an extension of Behrt, uses a hierarchical structure to process long sequences of medical data more efficiently. Furthermore, Med-BERT (Rasmy et al., 2021) modifies the pre-training task to include the prediction of length of stay and uses a combination of ICD-9 and ICD-10 codes to predict diabetes and heart failure. ICD-9 and ICD-10 are two different versions of disease classification. Proposed in 1979, ICD-9 comprises $14,000$ codes covering diagnoses and procedures. The codes are mainly numerical and fairly general. Adopted in 1990 and implemented in many countries in the early 2000s, ICD-10 is much more detailed, with around $70,000$ diagnostic codes. It provides a much more precise description of diseases and their symptoms. HiTANet (Hierarchical Time-aware Attention Network) (Luo et al., 2020) incorporates a temporal vector to represent the time elapsed between consecutive visits, combined with the embedding of the original visit to predict future diagnoses on three disease-specific databases. Finally, RAPT (RepresentAtion by Pre-training time-aware Transformer) (Ren et al., 2021) integrates an explicit duration vector with additional pre-training tasks such as similarity prediction and reasonableness checking to address issues of insufficient data, incompleteness, and the typical short sequences of EHR data. RAPT is evaluated for predicting pregnancy outcomes, risk periods, as well as diagnoses of diabetes and hypertension during pregnancy.

2.2 Validation of Self-Attention Links

Among the studies that use Transformer-type architectures on electronic health record (EHR) data, those that evaluate model performance by validating the self-attention links learned by the model fall into two groups. The first category includes works that assess the relevance of self-attention weights through a few selected examples. Among these works, the authors of LSAN (Ye et al., 2020), using a hierarchical attention module, randomly select samples to analyze which symptoms receive the most attention during each visit for risk prediction. Others, such as the authors of Behrt (Li et al., 2020), Med-BERT (Rasmy et al., 2021) and (Meng et al., 2021), use the *bertviz* (Vig, 2019) tool to visualize interactions between diagnoses with significant self-attention weights. This tool allows to visualize self-attention links between pairs of elements in a sentence, by choosing from the attention heads and layers of the model.

The second category includes work that modifies the representation of input data, making self-attention weights more interpretable. For example, (Dong et al., 2021) represent data as graphs linking domain concepts. This modification of the data representation improves the explainability of the attention mechanism, as it relies on the attention weights assigned to each graph instance and not just on the direct relationships between inputs and outputs. Similarly, (Peng et al., 2021) introduce ontologies as input data, demonstrating that it is possible to obtain more interpretable medical codes links.

Theses works aims to interpret and validate model learning through self-attention, but experiments in the EHR field are often limited to validating performance through manually evaluated visual examples. In this work, we propose a method that evaluates the learning of self-attention links by representing them as a graph and comparing them to a ground truth also represented as a graph. To represent self-attention links as a graph, we first extract these weights (Section 3.1) during inference of a Behrt (Li et al., 2020) model, by choosing a specific layer. These weights show the attention that each token gives to every other token in the same sequence. In parallel with this collection of data for all sequences, we identify the most influential tokens for prediction, by analyzing their gradient (Section 3.2). We then use these information to construct a directed graph (Section 3.3). In this graph, the tokens of importance are the source nodes, and they are connected to the other tokens to which they are linked in the sequences. We also add self-attention links between tokens that are linked to those identified as important, illustrating the interactions and self-attention weights between the different tokens playing a primary or secondary role in the prediction made by the model. Finally, we evaluate the graph by measuring the weight of directed edges common to those of a graph representing ground truth (Section 3.4).

3 METHODOLOGY

Figure 2 illustrates the different steps of our methodology.

3.1 Creation of the Global Attention Matrix

Let $T = \{t_1, t_2, \ldots, t_V\}$ be a set (or vocabulary) of V distinct *tokens*. We consider a labeled dataset $X = (X_i, y_i)_{i \in [\![1;N]\!]}$ consisting of N sequences X_i and their

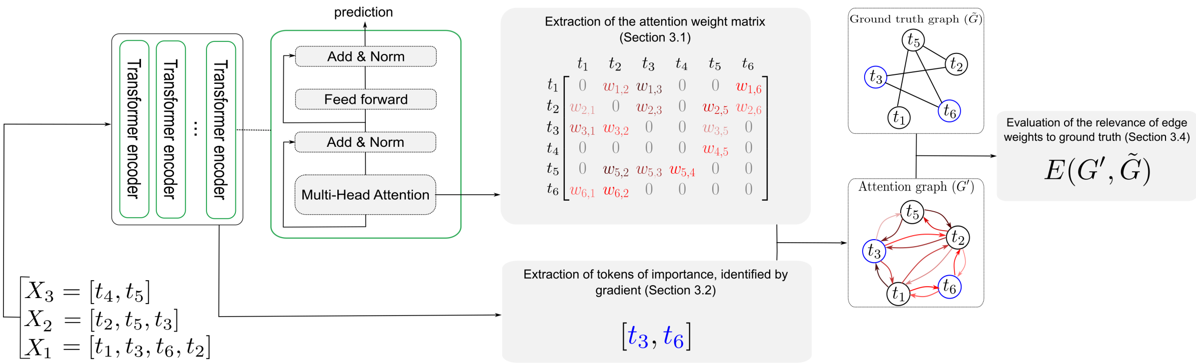


Figure 2: Stages of the proposed methodology: from the sequences given as input to a Transformer, we identify tokens of importance by gradient analysis. A global attention matrix is constructed in which each token assigns a weight (denoted w) to all other tokens in a global vocabulary, provided that both tokens coexist in the same sequence. Then, we extract a self-attention subgraph G' by starting with the important tokens (blue nodes) and adding all the tokens (black nodes) to which they are linked in the global attention matrix. A directed edge linking two nodes in G' is weighted by the self-attention weight that the source node assigns to the target node. We evaluate the relevance of the self-attention weights learned by the model using the evaluation function E, which compares the attention graph G' with the graph representing ground truth, denoted $\tilde{G}$.

associated ground truth y_i. Specifically, each X_i is a sequence of tokens $(x_1, \ldots, x_{z_i})$, where $z_i \in \mathbb{N}$ and $\forall j \in [\![1, z_i]\!], x_j \in T$. We feed each sequence X_i into a Transformer trained to predict $\hat{y}_i$. If the model's prediction $\hat{y}_i$ matches the true label y_i, we retrieve the attention matrix A_i of size $z_i \times z_i$ during the processing of X_i through the model:

$$A_i = \begin{bmatrix} a_{1,1} & a_{1,2} & \cdots & a_{1,z_i} \\ a_{2,1} & a_{2,2} & \cdots & a_{2,z_i} \\ \vdots & \vdots & \ddots & \vdots \\ a_{z_i,1} & a_{z_i,2} & \cdots & a_{z_i,z_i} \end{bmatrix} \tag{1}$$

where each element $a_{m,n}$ represents the self-attention that the token x_m in the sequence X_i gives to the token x_n in the same sequence. Specifically, in a Transformer layer, the self-attention $a_{m,n}$ is calculated by projecting x_m into a query vector $\mathbf{Q}_m = W^Q x_m$ and x_n into a key vector $\mathbf{K}_n = W^K x_n$, where, W^K and W^Q represent the learned weight matrices. These query and key vectors are used to compute a raw self-attention score via a dot product, which is then divided by the dimension of the key vectors (the size of the embeddings used to represent each token in the key space). Finally, this normalized score is passed through a *softmax* function that converts it into probabilities, resulting in :

$$a_{m,n} = \frac{e^{\left(\frac{\mathbf{Q}_m \cdot \mathbf{K}_n}{\sqrt{d_k}}\right)}}{\sum_{l=1}^{z_i} e^{\left(\frac{\mathbf{Q}_m \cdot \mathbf{K}_l}{\sqrt{d_k}}\right)}} \tag{2}$$

where z_i is the total number of tokens in the sequence X_i. Note that the self-attention $a_{m,n}$ in the matrix is calculated as the mean of the attention that token x_m gives to token x_n in all the attention heads of the selected layer.

Once we've retrieved the self-attention weights for each peer in each sequence, we aggregate these weights into a global attention matrix G of size $(V \times V)$ where V is the size of the token vocabulary T. Finally, the matrix G is nothing other than an adjacency matrix representing the self-attention links between all tokens. This matrix lists the values of the self-attention weights of all possible pair links among all tokens in the global vocabulary. Specifically, G synthesize the attention that each token t_m gives to each other token t_n across all analyzed sequences. For each pair of tokens (t_m, t_n), we identify all occurrences of these tokens in different sequences and accumulate the corresponding self-attention values for these tokens from the A_i matrices associated with each sequence. We collect these values into a set S_{mn}:

$$S_{mn} = \{a_{m',n'} \mid x_{m'} = t_m, x_{n'} = t_n, \\ m, n \in \{1, \ldots, V\}, m', n' \in \{1 \ldots, z_i\}\} \tag{3}$$

Each element $G[m,n]$ of the matrix is then calculated by taking the median of these values from the set S_{mn}:

$$G[m,n] = \text{Median}(S_{mn}) \tag{4}$$

Note that we choose to take the median value to avoid potential outliers. Finally, $G[m,n]$ captures the level of attention that each token t_m gives to every other token t_n across all sequences, reflecting the central tendency of the intensity of interaction between any pair of tokens in the dataset.

3.2 Identification of Important Tokens

For each sequence X_i where the model correctly predicts the label $\hat{y}_i$, we recover the gradient $\Delta(x_j)$ of each token x_j in X_i by performing a backpropagation pass. The gradients allow us to measure the influence of each token on the prediction. Knowing that the model makes a good prediction, gradients with higher values indicate a more significant contribution to the model's decision (Simonyan et al., 2014). For each token in the vocabulary T that appears in at least one correctly predicted sequence, we calculate the median importance of the gradients associated with that token.

Finally, we select a predefined number g of the most important tokens according to these median gradient measures, thus identifying those tokens that most consistently and significantly influence the model's correct predictions.

3.3 Self-Attention Graph Generation

We aim to construct a self-attention graph G' that represents the interactions between tokens as learned by the model. In other words, we extract a subgraph from the global attention matrix by selecting the relationships between a chosen set of tokens (nodes). In this section, we explain how we select the nodes of the graph.

To create an interpretable and comparable graph, we use the g tokens with the most significant gradients as the initial nodes of G'. Then, we expand this initial set by adding any token t_n from the global vocabulary T, for which the self-attention $G[m,n]$ is non-zero, where the token t_m or t_n belongs to the initial set of g tokens of importance. Thus, the set of nodes in G' includes the initial g tokens and all the tokens directly linked to them, with their associated median self-attention weights. We construct a directed graph where each pair (t_m, t_n) among the nodes of G' is connected by a directed edge from t_m to t_n if $G[m,n]$ is non-zero. The directed edges are weighted by the corresponding values of G, which quantify the intensity of self-attention t_m gives to t_n.

3.4 Evaluation of the Self-Attention Learned by a Model

We want to evaluate in an automated way the quality of the self-attention connections between tokens learned by an attention-based model. To do this, we compare these connections to a reference, represented by a graph $\tilde{G}$. For our experiments we have implemented a protocol for the creation of the reference graph by medical experts, detailed in Section 4.4. This ground-truth graph, $\tilde{G}$, contains the same nodes as the graph G' because we want to evaluate the interactions (directed edges) and not the tokens (nodes), which depend essentially on the sequences used. We wish to evaluate whether the model has learned a good distribution of self-attention weights compared to established expertise. For this, we introduce an evaluation method that takes into account the weight of edges, which is not the case for classical evaluation measures such as precision or recall. Evaluation is performed by calculating the difference between the weighted proportion of G' directed edges common to $\tilde{G}$ and the weighted proportion of G' directed edges not common to $\tilde{G}$. The evaluation function, which we call E, is calculated as follows:

$$E(G', \tilde{G}) = w_{in} - w_{out} \tag{5}$$

where:

- $w_{in} = \frac{\sum_{(m,n)\in G'\cap\tilde{G}} w_{mn}}{\sum_{(m,n)\in G'} w_{mn}}$, is the weighted proportion of directed edges in the graph G' that are also present in the ground truth $\tilde{G}$, i.e. the number of G' directed edges included in $\tilde{G}$ weighted by their weight and normalized by the weighted number of directed edges in G'.
- $w_{out} = \frac{\sum_{(m,n)\in G', (m,n)\notin\tilde{G}} w_{mn}}{\sum_{(m,n)\in G'} w_{mn}}$, is the weighted proportion of directed edges in G' that are not confirmed by $\tilde{G}$.

The evaluation function E measures the alignment between the graph G' and the ground truth $\tilde{G}$. It ranges from -1 to 1, where a score of 1 is reached when all directed edges of G' are included in $\tilde{G}$, and -1 when no directed edges are included. Scores between 0 and 1 indicate that directed edges included in $\tilde{G}$ are more heavily weighted than those not included, reflecting a predominance of matches. Conversely, scores between -1 and 0 indicate that directed edges not included in $\tilde{G}$ are more heavily weighted, reflecting a predominance of mismatches.

4 EXPERIMENTS

We evaluate our method using an attention-based model, trained by the *Lab Santé* of the *Direction de la recherche, des études, de l'évaluation et des statistiques* (Drees [2]). To test the validity of the graphs generated from self-attention weights and links, we set up a protocol for creating ground truth graphs in collaboration with the medical experts in the department.

[2]https://drees.solidarites-sante.gouv.fr

4.1 Model

We wish to study the learning of a model based on attention mechanisms, specifically adapted to the analysis of medical data. For our experiments, we use the model Behrt, a variant of BERT, trained on the task of predicting patient diagnoses during future hospital visit, based on a historical sequence of visits.

4.1.1 Data

The data on which the model was trained comes from the MCO (*Médecine, Chirurgie, Obstétrique*) tables of the PMSI (*Programme de Médicalisation des Systèmes d'Information*) of the SNDS. Each hospital visit is characterized by a set of diagnoses, including a principal diagnosis and, where applicable, a related diagnosis, as well as several associated diagnoses, which enrich the context of the principal diagnosis.

4.1.2 Training Task

The model is trained on a multi-class and multi-label classification task. This means that the label to be predicted can contain several different classes. The classes are represented by 2053 diagnoses coded according to the 10th revision of ICD, which is the list of codes that classify diseases and medical problems. The model training process is divided into two distinct phases to refine the predictive capabilities of the model, specializing it to meet the specific requirements of the medical field:

1. **Prediction of masked words**, where the model learns to identify and restore hidden elements in the training data.
2. **Fine-tuning of the pre-trained model** to specifically adapt it to the task of predicting diagnoses for upcoming hospital visits.

The training of the model for masked word prediction was conducted on individuals having more than 2 hospital visits and at least 3 diagnostic codes, drawn from two samples. A random sample of 4% of the SNDS data covering the period from 2008 to 2017, and a sample considering all SNDS data from 2018 to 2021. The dataset for the masked word prediction contains $14,59M$ samples. The training of the model for predicting diagnoses of the next hospital visit is carried out on individuals having at least 4 visits in their medical history, using the same datasets as the first phase. The dataset for the fine-tuning, i.e the prediction of the next hospital visit contains $5,94M$ samples. In both datasets, the minimum numbers of visits and codes in the sequence are imposed to ensure that the training sample contains sufficiently diverse medical paths and thus avoid overfitting.

4.2 Use Cases

We apply our method during the model inference phase, retrieving the medical histories of individuals for whom the model has correctly predicted the next visit, i.e. the diagnosis to be predicted is in the top 2 of predictions. We ensure that the other diagnosis in the top 2 is contextually related to the predicted diagnosis, reinforcing the relevance of our interpretation of importance gradients. We are working on two distinct use cases, based on different samples of test data. These use cases concern the prediction of incident diagnoses, meaning that the diagnosis to be predicted does not appear in the input sequence. This approach makes it possible to precisely analyze the influence of previous diagnoses on predictions.

4.2.1 Use Case of Childbirth

The class *childbirth* includes the following ICD10 codes: (**O80**) single spontaneous delivery; (**O81**) single delivery by forceps and suction cup; (**O82**) single delivery by caesarean section; (**O83**) other assisted single deliveries; and (**O84**) multiple deliveries. We select 2000 individuals for whom the visit to be predicted contains a label of the *childbirth* class, which is not in the sequence we give as model input. On the sample used, the model makes a good prediction for 190 individuals.

4.2.2 Use Case of Hypertensivity

The *hypertensivity* is defined by the following ICD10 codes: (**I10**) essential hypertension; (**I11**) hypertensive heart disease; (**I12**) hypertensive nephropathy; (**I13**) hypertensive cardionephropathy; and(**I15**) secondary hypertension. As in the case of childbirth, we randomly select 2000 individuals for whom the visit to be predicted contains the diagnosis I10 and none of the *hypertensivity* class labels is in the sequence corresponding to the medical history. On the sample used, the model makes a good prediction for 514 individuals.

4.3 Generation of Graph G' from Behrt in Inference

For each use case, the creation of the graph begins by retrieving the attention matrices for each individual, taken from the last layer of the Behrt model. Next, we build a global median attention matrix of dimensions 2053×2053, where 2053 represents the number of possible diagnoses. We also extract the gradient for each diagnosis from the sequence representing an individual's medical history, which we give as input to the model. This enables us to identify, for each individual, which diagnoses most influenced the prediction. We then calculate the median of the gradients per diagnosis.

For both use cases and to preserve confidentiality, we limit ourselves to the study of diagnoses or pairs of diagnoses present in at least five distinct medical pathways. This method allows us to maintain anonymity while preserving analytical relevance. Consequently, some diagnoses selected from the g diagnoses of importance may not appear in our graph if their connections with other diagnoses do not appear in the required minimum of five distinct medical pathways. Similarly, a connection between two diagnoses will not be visible in the graph if the pair of diagnoses does not appear in at least five distinct sequences. Thus, for both use cases, the number of significant diagnoses identified by the median gradient value is arbitrarily chosen so that the generated graph contains enough directed edges.

4.3.1 Use Case of Childbirth

We select the 10 most influential diagnoses according to the median value of their gradient (represented by blue-bordered nodes in Figure 3a). From these diagnoses, we extract the self-attention subgraph G' that links important nodes to other associated nodes in the global attention matrix, as well as links between added nodes (nodes that are not part of the set of importance diagnoses). Figure 3a illustrates the overall graph showing the self-attention relationships between the importance diagnoses, the diagnoses to which they are connected in the global attention matrix, and the links between these diagnoses. More precisely, an directed edge from node A to node B in the same graph is weighted by the median self-attention that A gives to B. The weight is represented by the color of the directed edge.

4.3.2 Use Case of Hypertensivity

We identify the 46 most significant diagnoses according to the value of their gradients. As with the childbirth use case, these diagnoses are then connected to the other tokens associated with them in the global attention matrix, and the directed edges of the graph are weighted according to the self-attention weight. The graph for this use case is shown in figure 3b.

[3] https://icd.who.int/browse10/2019/en

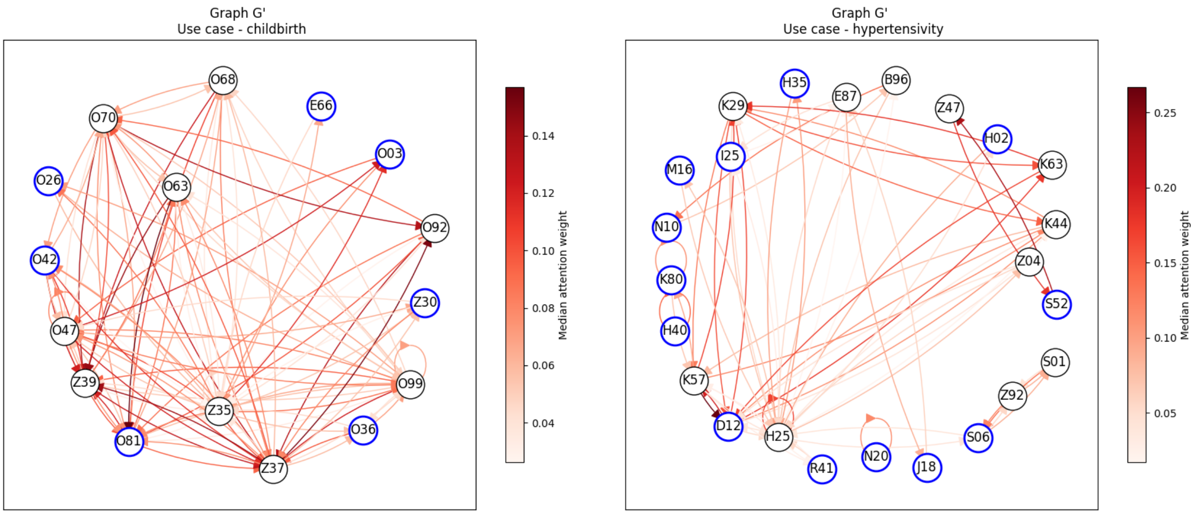
4.4 Creation of the Ground Truth Graph $\tilde{G}$

To interpret the links between diagnoses learned by the Behrt model through the mechanics of attention, we want to compare them with a ground truth, which translates into medical expertise. Self-attention, although significant in our model, has no direct and obvious correspondence in the medical context. In order to validate or invalidate these links, we have designed a protocol aimed at healthcare professionals, involving the creation of a graph of relationships between diagnoses. This graph is designed to be undirected and unweighted.

The protocol is based on two lists of diagnoses: the first, called ”gradients”, contains the diagnoses we have identified as important for prediction. The second, called ”other”, includes diagnoses that are related to the ”gradient” diagnoses according to the global attention matrix. To produce a graph that faithfully reflects the clinical reality of the two use cases presented, we called on the expertise of two Drees medical experts to form clusters. We specifically asked them to link each diagnosis from the ”other” list to one or more diagnoses from the ”gradient” list, taking into account the existence of a contextual correlation between them. This correlation may concern elements such as comorbidity, causality, impact on treatment, clinical implication, or coding frequency.

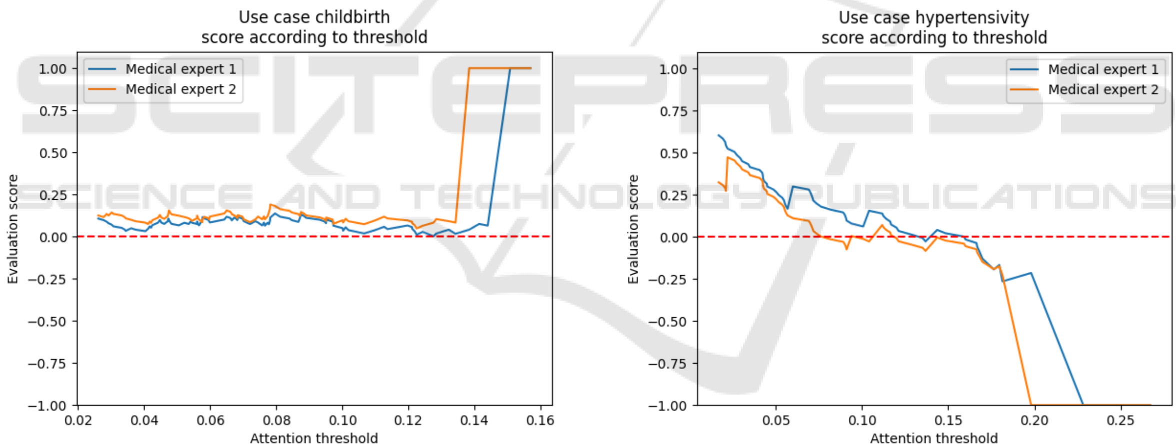
4.5 Evaluation of G' Relative to $\tilde{G}$

We evaluate the self-attention weights of the graph G' in relation to the ground truth $\tilde{G}$ by calculating $E(G', \tilde{G})$. Because G' is directed, and $\tilde{G}$ is not, we consider the edges of $\tilde{G}$ to be bidirectional edges. The aim is to analyze G' according to different thresholds that determine which directed edges are taken into account. More specifically, we aim to determine whether there is a threshold where the directed edges of G' in common with $\tilde{G}$ are correctly identified by the model as being significant, i.e. the weight of these directed edges is greater than that of directed edges not included. For each threshold established, we consider only those directed edges of G' whose weight exceeds that threshold. We then remove the isolated nodes from G' and keep the same nodes in $\tilde{G}$. The results of this evaluation, depending on the thresholds chosen, are presented in Section 5.



(a) (b)

Figure 3: Graphs obtained from our approach applied to the Behrt model in inference. The visualizations were generated using the *NetworkX* python package. (a) use case of childbirth, (b) use case of hypertensivity. Nodes with a blue border are diagnoses identified by the gradient as being important for prediction. Nodes with a black border are the diagnoses to which the importance nodes are linked in the global attention matrix. An directed edge from node A to node B has a color corresponding to the median weight of self-attention that A gives to B. Descriptions of ICD10-coded diagnoses in the nodes are referenced online[3].



(a) (b)

Figure 4: Curves illustrating the evolution of the evaluation score as a function of the self-attention threshold used to select directed edges in the G' graph. (a) corresponds to use case of childbirth, and (b) to use case of hypertensivity. In both figures, the blue curve represents the evaluation of the graph in relation to the medical expertise of the first doctor, while the orange curve reflects the evaluation in relation to the second doctor. A red dotted line located for score=0 is included to facilitate visualization of evaluation scores that become negative.

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5 RESULTS

We are testing our evaluation method on two use cases: the prediction of a diagnosis signaling childbirth, and a case revealing a diagnosis of essential hypertension. To do this, we evaluate the graph generated from the information extracted during inference phase of the Behrt model, by comparing it with ground truths obtained via the protocol described in Section 4.4 and involving two medical experts. This evaluation consists in computing the difference between the weighted proportion of directed edges common to the ground truths and those not included, i.e. those not validated by the ground truths. We adjust the threshold above which directed edges are considered in the graph G' to determine whether, above a certain threshold, directed edges included in the ground truths have a more significant weight than those excluded. This allows us to determine whether a specific threshold produces a graph that most closely approximates the ground truth.

The curves evaluating the score of G' in relation to ground truths are shown for each use case in Figure 4. For the case of childbirth (see Figure 4a), we observe that above a threshold of 0.13 or 0.15, depending on the ground truth, the score reaches 1. This indicates that all the directed edges of G' are included in $\tilde{G}$, confirming the existence of a threshold beyond which the directed edges correspond precisely to the ground truth and demonstrating that the model correctly assigns high self-attention weights to the relevant directed edges. Before this threshold, the score remains positive but does not exceed 0.25, suggesting that, although some directed edges are not included in the ground truth, their influence is relatively minor.

On the other hand, in the case of hypertensivity (see Figure 4b), the curves show a constant decay, meaning that the higher the directed edge selection threshold, the fewer directed edges are in common with the ground truth, or their weight is less than those excluded. These results indicate that, in this use case, the model fails to pay sufficient attention to diagnosis pairs validated by the expert.

6 DISCUSSION

We develop a method for automatically evaluating the links between tokens learned by an attention-based model, using the Behrt architecture, trained by the *Lab Santé* (Drees) on SNDS data. We analyze the learning of the model on a task that can be evaluated by an expert: the prediction of a diagnosis. More precisely, the model we use is trained to predict the next hospital visit from a sequence of previous visits, which does not contain the diagnosis to be predicted, which we call an incident diagnosis. We graphically represent the model's learning by linking diagnoses identified as important by their gradient to the diagnoses to which they are linked via the self-attention learned by the model. The representation we propose makes it easier for medical experts to understand how the Behrt model is learned. It enables the analysis of self-attention links between tokens, which can be compared to correlations between diagnoses in the medical field.

Our approach enables a more granular assessment of model learning than would be possible with global measures such as precision or recall. Indeed, the framework we propose facilitates visualization and evaluation of the diagnostic links learned by the model, and enables learning to be adjusted according to these observations. Although the model does not achieve a high recall rate - correctly diagnosing 190 out of 2000 individuals in the case of childbirth and 514 out of 2000 in the case of hypertensivity - our approach is applied to determine whether these results are the result of overfitting. Analyses reveal that the model establishes more relevant diagnostic links for childbirth than for hypertensivity, which is surprising given the better recall rate observed for hypertensivity. This anomaly is interpreted as being due to the complexity of the hypertensivity case, which presents a wide variety of diagnostic pathways that can lead to correct predictions. These results demonstrate the added value of our approach, whose analysis creates a direct link between the training data used and the performance obtained, enabling potential adjustment of the sample used.

In our experiments, we developed a protocol for creating a ground truth graph, which allows us to evaluate the graph of self-attention links learned by the model. The curves shown in Figure 4 indicate that the evaluation score of the model graph, relative to the ground truth graph, follows the same trend, independently of the medical expertise being compared. This finding suggests that our proposed protocol succeeds in establishing a ground truth that reflects shared medical knowledge, thus reinforcing the validity of the established ground truth as representative of general medical expertise. The protocol for establishing the ground truth does not take into account the weighting of edges, as there is no direct and obvious correspondence with self-attention in the medical context. In the future, we would like to develop a method to weight the edges established by medical expertise, in order to more accurately evaluate the self-attention weighting adopted by the model.

Finally, the proposed method offers an accurate assessment of model learning based on attention mechanisms, which is fundamental in the medical field. Indeed, understanding how the model learns is crucial to being able to use its predictions to make informed decisions.

7 CONCLUSION

Our method aims to validate the learning of models based on self-attention mechanisms by representing the learned links as graphs and evaluating their relevance to a graph that represents the ground truth. This approach enabled us to gain a better understanding of how a BERT-type model works, specifically trained to predict the diagnosis of the next hospital visit based on a series of previous visits. Our experiments on two distinct use cases revealed that the case where the model showed better initial performance established less relevant diagnostic links than in the case where the model appeared a priori to perform less, underlining the importance of a detailed analysis of learned relationships.

We have also developed a method for creating a ground truth from a simple-to-implement protocol. Although we have considered ground truths defined individually by different medical experts, a future approach could be to unify these various truths into a single one. Furthermore, the protocol for establishing the reference graph does not take into account the weighting of edges, as there is no direct correspondence with self-attention in the medical context. In the future, we would like to develop a method for weighting the edges established by medical expertise, thus enabling a more accurate assessment of the self-attention distribution assigned by the model.

To extract a subgraph from the global attention matrix, which we call the self-attention graph, we start with g tokens considered important for prediction based on their associated gradients. The number g is chosen to have a graph with enough edges to evaluate. Subsequently, we would like to extract the graph using a less arbitrary initialization, for example by extracting weakly connected components based on a self-attention threshold in the global attention matrix. This would also allow us to evaluate the different components derived from the global attention matrix against those from a richer reference graph.

To generate the graph, we used the self-attention weights of the last layer of the model. However, we plan to explore the weights of other layers in the future and design a method for integrating the attention of all layers, in order to better evaluate learning. Furthermore, the self-attention weight between two tokens is calculated by averaging the self-attention weights from all attention heads in the last layer. In our future work, we plan to analyze each attention head individually to examine whether the associated weights may have distinct interpretations in the medical context. Finally, we aggregate the self-attention weights between two tokens by calculating the median of these weights in all sequences combined. In future work, we'd like to study the impact of the choice of aggregation operation.

Finally, the results obtained showed that our approach enables a different performance analysis to that obtained with global evaluation measures. Indeed, in the two use cases studied, our method revealed biases linked to the training data, which were not detectable with recall measures, for example. In this way, our approach facilitates understanding and confidence in the predictions made by a model, thanks to an automatic but thorough analysis of its learning.

ACKNOWLEDGEMENTS

We thank Milena Suarez Castillo and Javier Nicolau for allowing this collaboration, the Lab Santé team for the model developpement and the medical experts Diane Naouri, Albert Vuagnat, and Constance Prieur for their valuable expertise and the time dedicated to this work. Their active participation in the validation exercises greatly contributed to the quality of our study.

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