Toward automatic comparison of visualization techniques: Application to graph visualization

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Abstract

Many end-user evaluations of data visualization techniques have been run during the last decades. Their results are cornerstones to build efficient visualization systems. However, designing an evaluation is always complex and time-consuming and may end in a lack of statistical evidence. The raising of modern efficient computer vision techniques, such as deep convolutional neural networks, may help visualization researchers to adjust their evaluation hypothesis and thus reduces the risk of failure. In this paper, we present a methodology that uses such computer vision techniques to automatically compare the efficiency of several visualization techniques. The basis of our methodology is to generate a set of images for each compared visualization technique from a common dataset and to train machine learning models (one for each set and visualization technique) to solve a given task. Our assumption is that the performance of each model allows to compare the efficiencies of the corresponding visualization techniques; as current machine learning models are not capable enough to reflect human capabilities, including their imperfections, such results should be interpreted with caution. However, we argue that using machine learning-based evaluation as a pre-process of standard user evaluations should help researchers to perform a more exhaustive study of the design space and thus should improve the final user evaluation by providing better test cases. To show that our methodology can reproduce, up to a certain level, results of user evaluations, we applied it to compare two mainstream graph visualization techniques: node-link (NL) and adjacency-matrix (AM) diagrams. We partially reproduced a user evaluation from Ghoniem et al. using two well-known deep convolutional neural networks as machine learning-based systems. We generated graphs associated to their pair of NL and AM diagrams to train our networks for automatically solving three standard low-level tasks on graphs. Our results show up that Ghoniem et al. results can be reproduced automatically at a larger scale with our system.

1 Introduction

Information visualization has now been established as a fruitful strategy in various application domains for exploration of large and/or complex data. When designing a new visualization technique, it is necessary to assess its efficiency compared to existing ones. While computational performances can be easily evaluated, assessing user performance is more complicated. This is usually achieved by carrying out a user evaluation that compares the techniques on one or several tasks \([1, 3, 19, 20, 23, 34–36]\). During such a study, a population of users is asked to solve several times the same task using various input data presented with different visualization techniques or different variations of a technique. Experimental results (e.g., accuracy or completion time) are then statistically validated to confirm or refute some preliminary hypothesis. Completing a user evaluation can become time-consuming as the number of techniques, the considered dataset, and the number of tasks increase. As that may bias the experimental results due to loss of attention or fatigue, it is necessary to maintain reasonable the completion time of the entire evaluation. To that end, one usually tries to keep reasonable the number of experimental trials \([38]\) by reducing the number of evaluated techniques, the number of tasks and/or the dataset. This is one of the strongest bottlenecks of user evaluations as visualization designers have to reduce the explored design space to a few visualization techniques without any strong evidence. This paper presents a strategy to overcome this issue.

We introduce a new methodology for automatically comparing visualization techniques. As no user is involved in such an evaluation, visualization designers could assess the relative efficiencies of several visualization techniques, or variations of one, before carrying out a formal user evaluation. Such an automatic evaluation could therefore be considered as a pre-process of a real user evaluation. Since the publication of the AlexNet in 2012 \([26]\), and its outbreak of performance in the ImageNet challenge \([25]\), deep neural networks systems \([28]\) are used in more and more scenarios (e.g., automatic language translation, instance segmentation, image captioning, speech generation and synthesis) and outperform well established state-of-the-art methods. Behrisch et al. \([1]\) mention, in their survey on quality metrics in visualization, that using supervised machine learning approaches, such as deep learning, is a promising direction for evaluating the quality of a visualization. Haehn et al. \([21]\) and Haleem et al. \([22]\) made use of such systems in an information visualization context and showed that these techniques can be...
Figure 1: Illustration of our methodology. First steps consist in generating data and their representations with the visualization techniques to compare. Next steps consist in training models, selecting the best ones and evaluating them on unseen data. Finally, the efficiencies of the visualization techniques are compared using usual statistical methods as for any quantitative user evaluation.

largely beneficial to our community. Our methodology also takes advantage of these computer vision techniques to automatically assess the efficiency of a visualization technique for a given task. The basis of our methodology is first to generate a set of images for each compared visualization technique from a common dataset and then, to train models (one for each set and visualization technique) to solve that task. We assume that if model $M_A$ trained with visualization $A$ is able to perform a task more accurately than model $M_B$ trained with visualization $B$, there is an efficiency difference between technique $A$ and $B$ to solve that task. To demonstrate the effectiveness of our methodology, we have partially reproduced a previous user evaluation [19, 20] comparing node-link diagram (NL) and adjacency matrix diagrams (AM) for three counting tasks. That evaluation involved 27,000 graphs and twice as many images. Our hypothesis is that trained models should reproduce existing results: that AM outperforms NL for these tasks.

The main contribution of this paper is a new methodology that relies on machine learning to automatically compare the efficiencies of visualization techniques. It is aimed to be used as a pre-process of a standard user evaluation to help researchers to perform an exhaustive study of the design space and to ease the selection of visualizations to be evaluated by users. We validated our methodology by partially reproducing the results of Ghoniem et al. [19, 20].

The reminder of this paper is organized as follows. Section 2 presents related works with a focus on machine learning for counting, machine learning for information visualization and user evaluation of graph visualization techniques. Section 3 describes the proposed methodology and its different steps. Section 4 describes the experimental evaluation made to assess the pertinence of the methodology and its results through a use-case. Section 5 discusses the obtained results. Finally, Section 6 draws conclusions and present directions for future works.

2 Related works

Human and computer vision algorithms have been compared [16, 44]; in average, machine learning algorithms are better when the set of images focuses on a given task [17] while humans outperform when bias (e.g., distortion) are introduced in the images [15]. The proposed method is related to the use of machine learning for information visualization and machine learning for counting and has been validated in the context of evaluation of graph visualization. The remaining of this section focuses on these three points.

2.1 Machine learning for information visualization

Graphical Perception. Heahn et al. [21] have reproduced Cleveland and McGills settings [13] with four different neural networks. Their goal was to show how these networks compare to human. Their result is that CNN perform better or equally than humans for almost all the tasks, but they cannot estimate edge length ratio properly. In that work MultiLayer Perceptron (MLP), LeNet [29], VGG [43] and Xception [11] networks have been tested. In each case, results were better if the networks were completely retrained specifically for a specific task. We borrowed these results to run our experimentation and thus we use completely retrained CNNs.

Readability of Force Directed Graph Layouts. Haleem et al. [22] work is the most similar in spirit to ours. They proposed to use handcrafted CNN (inspired by VGG) in order to find properties of force directed layouts in node link diagrams. While the focus of that research is to design an optimized CNN architecture for that particular task, our methodology relies on standard model architectures. We assume that these models, designed by the
machine learning community, are efficient \cite{21}, and we make directly use of them to compare various visualization techniques.

### 2.2 Machine learning for counting

In this paper, we aim to compare several counting tasks on two graph visualization techniques (see Section 4.1.1) using machine learning techniques. Recent advances in that domain have proven that such tasks may be automatically done but also provide some cues to set up our experimentation.

**Complete image versus patches.** Lempitsky and Zisserman \cite{31} propose a semi-supervised learning framework for visual object counting tasks. They recover the density function of objects in an image thanks to a linear transformation from the feature space that represents each pixel. A tailored loss function helps to optimize the weights of this linear transformation while the integration of the density function provides the number of objects. The method has been validated on cell counting on fluorescent microscopy images and people counting in surveillance videos. Other visualization methods are not exactly the same but achieve more than 90% of prediction on 100 real images of tomato plants.

**Group.** Studies showed that \cite{19,20} improve the former work by 20% with an approach based on CNNs in a boosting framework (CNN_{i+1} learns to estimate the residual error of CNN_{i}) and image patches. While that method improves the performances, we use full image search method in our experiment since we do not make any assumption on the size of the objects to be counted.

**Kind of objects to count.** Recent research also proved that deep networks may learn automatically the kind of graphical objects to count. Segui et al. \cite{22} estimate the count (up to 5) of even digits in an image. They show that the network can extract features that encode the objects to count whereas they have never been explicitly provided to the network. Another result is the one of Rahmoomanfar and Sheppard \cite{19}: they use a deep learning framework to count fruits in images. The originality of this work resides in the use of artificial images during the training while still achieving more than 90% of prediction on 100 real images of tomato plants.

Previous work on deep learning network already proved that if an image enables to count a certain kind of objects, it may be possible to learn it without any specific tuning. Therefore, for graph counting tasks, it may be possible to use the same learning technique on different visualizations without specific changes according to the way entities and relations are visually encoded.

### 2.3 User evaluation of graph visualization

User performance evaluations have been widely adopted by the visualization community to assess the efficiency of visualization techniques and comparing them \cite{27}. Realworld users’ tasks are generally of higher level, but can be decomposed into low-level ones. These low-level tasks are usually evaluated by quantitatively and qualitatively comparing the performances of users on visualization techniques (e.g. number of elements in the visualization or identification of an element according to some particular property). Evaluating the performance of a visualization technique for the involved low-level tasks therefore provides some cues about its efficiency for these high-level tasks. Moreover, solving high-level tasks may necessitate multiple, possibly linked, views using various visualization techniques as well as various interaction tools which make difficult the interpretation of the results (except for usability studies). Task taxonomies \cite{34,35,36} are powerful tools to identify relevant tasks by describing them in a structured manner that emphasizes their relative closeness.

We focus in this paper on the evaluation of the two most widely accepted graph visualization techniques: nodelink (NL) and adjacency matrix (AM) diagrams to show the effectiveness of our methodology. Many researches either try to improve one or the other by optimizing an aesthetic criterion or an objective function, or to identify some criteria of the visualization/data that can facilitate the task solving. For instance, studies of Purchase \cite{37} and Kobourov et al. \cite{25} compared the importance of some aesthetic criteria on user performance for tasks related to graph connectivity (e.g. length of a shortest path, the number of nodes to remove to disconnect the graph, or identify the neighborhood of a given node) in NL. Mueller et al. \cite{33} compared the impact of several node ordering algorithms on the readability of an AM. Concurrently, user evaluations have also been performed to compare the efficiency of the two visualization techniques \cite{11,19,20,23,34,35,36}. On the one hand, Ghoniem et al. \cite{19,20} evaluated these techniques on seven counting and connectivity tasks and concluded that NL performs better than AM for connectivity tasks when graphs are small and sparse while AM outperforms NL in all the others conditions. These results were later reproduced by the user evaluation of Keller et al. \cite{23} for similar tasks even with small graphs. In their evaluation, Alper et al. \cite{3} compared two variations of NL and AM for dynamic weighted graphs and concluded that AM performs better than NL for weight variations and connectivity tasks. On the other hand, Abuthawabeh et al. \cite{1} did not find any difference in term of user performance when considering higher level tasks of the software engineering domain. Sansen et al. \cite{41} compared four visual edge encodings in AM among which one corresponds to a NL where nodes have been duplicated for the path finding task. This evaluation showed very few significative differences between AM and their variation of NL. Somewhat contradictory results were as well obtained by other researches \cite{34,35,36}.

Okoe and Jianu partially reproduced two connectivity \cite{14} tasks out the seven tasks of \cite{19,20} with some modifications of the experimental setup. These modifications consisted in using a realworld dataset, ordering the matrix to emphasize the cluster structures and allowing node drag in the NL. Another important difference is the size of the involved population as running their experiment with an online system allowed them to recruit a larger number of participants. The results of that evaluation showed that RL outperforms AM on each tested task. A larger scale study has been presented by Okoe et al. \cite{15,36}. This evaluation explored a larger range of tasks as it included fourteen tasks classified into topology/connectivity, group and memorability tasks. That study showed that RL outperforms AM for topology/connectivity and memorability tasks while the contrary can be observed for group tasks. We believe that these contradictory results are mainly due to three aspects. First of all,
even though the evaluation protocols are similar, their slight differences (available interaction tools, wording of the questions) can drastically induce variations in the results. The second aspect relates to the populations involved in these studies. As their size (e.g., from few dozens in [19,20] to few hundred in [35,36]) and demographics varied (e.g., post-graduate student and researchers in computer science in [19,20] and Amazon Mechanical Turk users in [35,36]), the results can vary as well. The last aspect relates to the evaluation datasets as these evaluations are performed in distinct contexts and therefore use distinct datasets having distinct topological properties.

3 An Automatic Evaluation Methodology

The key idea of the proposed method is to use artificial intelligence (thanks to machine learning models) to solve a given task for each considered visualization technique to be compared. Then, the efficiency of these techniques can be evaluated by comparing the performance of their related models. While bio-inspired models [45] try to mimic human behavior, many of modern machine learning models do not perform like humans but rather try to perform better than them [13]. This implies that if such a model cannot solve a task on a visualization, it should be even more difficult for a human-being. Several important criteria for Human Computer Interface (HCI) field can be estimated using such machine learning models:

- **Learning convergence**: by comparing how fast a visualization can be understood by the model, one can do the hypothesis that it will be easier for humans. Such an hypothesis could then be used to set up a prototype and then run standard evaluations with humans.
- **Complexity of the task**: models have various structure complexity (number of layers, type of operations in the layers, etc...); by automatically checking the performance of several well-known models going from less complex to more complex, one can automatically evaluate the difficulty to solve a task with a specific visualization. Of course, once again, these results may only serve to build hypotheses that need to be confirmed by a human-based experimentation.
- **Accuracy of a visualization**: by measuring the number of good/bad results for a task, one can compare a visualization to another. Errors are usually present when there is some ambiguity in the visualization due to, for instance, cluttering issues. Modern machine learning-based models perform quite well here and thus one can assume that if the model cannot solve the ambiguity, it will also be hard or at least time consuming for a human-being.

Figure 1 describes our methodology while the rest of the section presents each block of our evaluation framework: the data generation, the images, tasks and ground truths, the model selection and the model evaluation and Performance comparison. It also presents which role is expected by the visualization experts.

3.1 Data generation

Our method should be applied in a context for which we know which tasks have to be handled on which visualizations techniques. Consequently, we should have a set of input data (that will be later visualized with the different techniques) associated to the expected answer. Such dataset of raw data can either be generated automatically using a data generation algorithm or collected from existing data source. Our experiment has shown that the data generation process requires a significant attention. Indeed, as we detail in the next sections, distribution of the data is of utmost importance: the more uniform the probability is, the easier the setup of evaluation and training is. It is not always easy or feasible to generate datasets respecting this constraint. As one of the key features of our methodology is the reproducibility of the evaluation, generated data can be stored and reused for any future experimentation. It enables the community to create test beds for comparisons of new visualization techniques with previous ones.

3.2 Images, tasks and ground truths

The second step consists in generating visual representations for each input data with each visualization technique. They will be used during the experiment. In our current framework, we only deal with static visualization and we do not enable interaction on the visualization. Thus, that step consists in generating static tagged images on which a model or a user should answer to a question (i.e., solve a task). We note $v_i = (img_i, grd_i)$ a data sample, where $img_i$ is the image (corresponding to a visualization technique) and $grd_i$ is the ground truth to be predicted among the sequence of all possible answers for a given task, noted $G$. As previously stated, generating a set $V = \{v_1, ..., v_n\}$ of samples for a given task is challenging as it has to follow a valid distribution. For instance, if the same value has to be predicted in 80% of the cases and a model has an accuracy of 80% for that task, it could mean that the model succeeded in detecting the bias in our experiment. Ideally, the distribution should verify the following property:

$$\sum_{i \in G, (img, grd) \in V} I\{i = grd\} = \sum_{i \in G, (img, grd) \in V} I\{j = grd\} = \frac{4}{5} \quad (1)$$

where $I\{a\} = \begin{cases} 1 & \text{if } a \\ 0 & \text{otherwise} \end{cases}$.

In other words, each ground truth of $G$ should appear the same number of times in $V$: its distribution should therefore be uniform. Such experiment is usually not feasible with users since the number of experimental objects is too large making the entire completion time unrealistic.

During a formal user evaluation, a first step is to let the user learns the visualization and the task on a training set. Automatic evaluation framework works similarly: the set $V$ is split into three sets called train (to learn the
model), validation (to select the best model across the epochs) and test (to evaluate the model) datasets; they are respectively noted \(V_{train}, V_{validation}\) and \(V_{test}\). Each of them should verify the property \(\{\}\) and thus initial set \(V\) must be large enough. In our experiments (see Section \[\]), we use a set \(V\) of 27000 samples (per visualization technique) due to computer memory limits but the larger the set \(V\) is the better it is.

### 3.3 Model selection

The model selection step consists in choosing the model that performs the best in \(V_{validation}\). It means that it has well learned with \(V_{train}\) and is able to generalize with the dataset \(V_{validation}\) (e.g., it does not suffer of over-fitting).

For that purpose, we apply standard learning methodology; in the case of deep neural networks-based models, first we train models during a fixed number of epochs (100 by default). To select the best model over the epochs, the performances of the model are evaluated, at the end of each epoch, using its predictions on \(V_{validation}\). For each epoch \(e\) and each \(v \in V_{validation}\), a prediction is the answer provided by the model and is noted \(\hat{y}_e(v) \in G\). We can then evaluate for each epoch the accuracy of the predictions regarding the ground truths. The accuracy is defined as follows:

\[
\text{accuracy}(y, \hat{y}) = \frac{\text{Card}(y)}{\text{Card}(\hat{y})}
\]

where \(y\) is the list of ground truths (i.e. \([\text{grd} | (\text{img}, \text{grd}) \in V_{validation}]\)) and \(\hat{y}\) is the list of associated predictions (i.e. \([\hat{p}_e(v) | v \in V_{validation}]\)). That metric, common in both the visualization and the machine learning communities, provides the percentage of exact predictions (higher is better).

During this step, we make sure that the selected model has effectively learnt how to solve the considered task. This is usually achieved by comparing the predictions of a model to random choices or computing evaluation metrics. In this work, we propose to use two metrics, called Matthews correlation coefficient (MCC) and coefficient of determination \(R^2\) respectively designed for classification and regression problems.

The Matthews correlation coefficient is defined as:

\[
\text{MCC}(y, \hat{y}) = \frac{\sum_{i,j} C_{ij} \cdot (\text{Card}(y_i)) \cdot (\text{Card}(\hat{y}_j))}{\sqrt{\sum_{i,j} C_{ij} \cdot (\text{Card}(y_i)) \cdot (\text{Card}(\hat{y}_j)) \cdot \sum_{i,j} C_{ij} \cdot (\text{Card}(y_i)) \cdot (\text{Card}(\hat{y}_j))}}
\]

considering the confusion matrix \(C\) (built from \(y\) and \(\hat{y}\)) of a \(K\) classification problem. This metric has the advantage of being insensitive to unbalanced datasets. A value of 1 represents a perfect prediction, 0 a random prediction and −1 a total disagreement between the prediction and the ground truth.

The coefficient of determination is defined as:

\[
R^2(y, \hat{y}) = 1 - \frac{\sum_{i=1}^{\text{Card}(y)} (y_i - \hat{y}_i)^2 / \sum_{i=1}^{\text{Card}(y)} (y_i - \bar{y})^2}{\sum_{i=1}^{\text{Card}(y)} (y_i - \bar{y})^2}
\]

where \(\bar{y} = \sum_{i=1}^{\text{Card}(y)} y_i / \text{Card}(y)\) 1 means that \(\hat{y}\) explains perfectly \(y\) (very good system), while 0 means the opposite (very bad system).

### 3.4 Model evaluation and Performance comparison

To evaluate the selected model performances but also to ensure that it generalizes well, we use \(V_{test}\) as input data. As the elements of \(V_{test}\) have not been previously processed during the learning and model selection stages, we can measure the capacity of the model to solve a task on an unseen image.

For each \(v \in V_{test}\), we compute \(p_e(V_{test})\) using the best epoch \(e\) found during the model selection stage. We note \(p_e(V_{test})\) the sequence of all predictions for the elements of the sequence \(V_{test}\). When comparing \(k\) visualization techniques (or variations), the \(k\) corresponding models provide \(k\) sequences of predictions to be compared. It is noteworthy to mention that the best epochs may be different for each model. Performance comparison consists in comparing the sequences of predictions of each model (i.e. each visualization technique) with the ground truths. For that purpose, we can use several metrics to evaluate each prediction and then we use standard statistical test (e.g. Wilcoxon signed rank, Kruskall Wallis) to determine if one of the predictions is significantly better than another one. In the experiment presented in Section \[\] we used four metrics, the accuracy that was defined previously and:

- **MSE (mean squared error):**

\[
mse(y, \hat{y}) = \sum_{i} \frac{|y_i - \hat{y}_i|^2}{\text{Card}(\hat{y})}
\]

That is a common regression metric in the machine learning community that considers the labels proximity (lower is better).

- **percent10:**

\[
\text{percent10}(y, \hat{y}) = \sum_{i} \frac{\text{Card}(y_i) \cdot 1\{9y_i - \hat{y}_i < -0.1y_i\}}{\text{Card}(\hat{y})}
\]

That metric is a variation of the accuracy that allows +/-10% of errors (higher is better).

- **delta10:**

\[
delta10(y, \hat{y}) = \sum_{i} \frac{\text{Card}(y_i) \cdot 1\{|y_i - 10 < \hat{y}_i < y_i + 10\}}{\text{Card}(\hat{y})}
\]

That metric is a variation of the accuracy as well that allows +/-10 units of errors (higher is better).

MSE, percent10 and delta10 are three regression metrics and may not be used for classification problems. While MSE allows to measure the distance of the predictions to their associated ground truths, percent10 and delta10 consider predictions that are close to their ground truths as correct. Even if percent10 and delta10 are similar, they also seem to have opposite limitations. While percent10 is more permissive when the predictions are associated to high-value ground truths than low-value ones, delta10 has the opposite behaviour. Both are therefore sensitive to the average value of the ground truths as well as their distribution.
3.5 Role of visualization experts

Our evaluation methodology permits to run experimentations without involving humans in the evaluation process. However visualization experts must stay in the loop even at the early stages of the process and play the same role as in formal user evaluations. In particular, the expert must set all the experimental parameters such as the visualization techniques to be compared, the considered tasks and hypothesis, the data generation model (or the collection of data) as well as the evaluation metrics. These experimental protocol parameters define the limitations of the methodology proposed in that paper, in the same way as for user evaluation. The results have therefore to be considered within these limitations.

Figure 2: Examples of (a) AM and (b) NL images for a graph of 50 nodes and density 0.2. As the area of AM representation is quadratic on the number of nodes, its nodes appear smaller than in NL.

4 Use case : experimental comparison of NL and AM

This section presents the experimental protocol we have applied to evaluate the proposed methodology (see Section 3) on a specific use case. It was mandatory to reproduce an existing user evaluation study that serves as a reference otherwise no conclusion about the effectiveness of our methodology could have been drawn. We therefore reproduced 3 tasks out of the 7 tasks of Ghoniem et al. [19, 20]. In the following, we describe the evaluation protocol, the technical details, the results and we discuss the main limitations of the study.

4.1 Evaluation protocol

4.1.1 Tasks, visualization technique and hypothesis

As previously stated, we decided to partially reproduce the user evaluation of Ghoniem et al. [19, 20]. In particular, we focus on its three first tasks that mainly relate to counting: (i) Task 0: exact count of the number of nodes; (ii) Task 1: exact count of the number of edges; (iii) Task 2: maximum degree of the graph. Task 0 and Task 1 are slight variations of the two first tasks of Ghonien et al. which consisted in providing estimates of the number of nodes and edges. Even if the model is trained to answer exact counts, during the next steps, estimates of the ground truths can be considered (see Section 3.4). Task 2 is a variation of the third task of Ghonien et al. as they considered identification of the node of maximum degree instead of the maximum degree.

Several studies [19, 20, 35, 36] have provided contradictory results about the efficiency of NL and AM. However, to the best of our knowledge, none of these results are related to these 3 tasks. It was to a certain extent mandatory in this study in order to validate our methodology as we expected our results to corroborate those of Ghoniem et al. [19, 20]. Our hypothesis is therefore that:

\[ H: \text{AM should outperform NL for each of the three tasks.} \]

4.1.2 Graph dataset

Similarly to Ghoniem et al. [19, 20], we used random graphs in this experiment. However, the number of graphs considered in our experiment is much larger. On the one hand, supervised learning methods necessitate a large training dataset and on the other hand, we have made the hypothesis that using many graphs would help to train models able to better generalize. When generating the graphs of this study, we took two parameters into account:

- the number of nodes which varies from 20 to 100 (we refer to this parameter as the graph size),
- the edge density as defined in [19, 20] which was set to 0.2, 0.4 and 0.6 and corresponds to \[ \sqrt{\frac{2|E|}{|V|}} \].
Figure 3: Description of the selected networks: LeNet on the left and VGG16 on the right. Operation are represented in rectangular shapes with their name and eventual parameters. Data (i.e., input/output of an operation) are represented by a rounded rectangle with the dimension of the underlying tensor when one example is given to the network. In our methodology, a model is trained for each triplet of model architecture, task to be solved and visualization technique.

There are $3 \times 81 = 243$ combinations of parameters. 100 instances are generated for each combination, which led to 24,300 graphs in total for training and validation. 2700 additional graphs are generated for test while trying to follow the same distribution as for the training and validation datasets. This leads to a total number of graphs of 27,000. Our machine learning platform constrained us to use a number of graphs multiple to the batch size (400 in our case due to the memory limits of the platform).
We are interested in verifying if we are able to learn the model, how they perform and how they compare between

As mentioned in Section 3, it is mandatory to determine whether the models were able to learn how to solve the
generation of graphs and their two representations is done by a tool written in C++. Graph drawing and
regression one as the goal is to predict a value (i.e. a class instead of a value) in order to generalize them for other tasks in the future. For the same reason, the output

Table 1: Summary of the number of parameters to train for each model configuration.

|        | Task 0      | Task 1      | Task 2      |
|--------|-------------|-------------|-------------|
| LeNet  | 218,523,668 | 238,598,968 | 218,523,668 |
| VGG16  | 166,126,372 | 186,201,672 | 166,126,372 |

4.1.3 NL and AM images datasets

In order to train (but also to validate and test) the models, we computed a 256 × 256 grayscale image for each combination of graph, task and visualization technique (NL or AM).

Concerning the NL diagram, nodes were represented by a circular shape, and each graph has been laid out with the GEM force-directed algorithm [15]. To facilitate the identification of nodes and edges, node size has been set to half the minimum distance between any two nodes in the resulting drawing. Concerning the AM diagram, we computed the ordering of nodes by using the Louvain clustering algorithm [8]. This emphasizes the community structures of the graph even if assessing such a topological information is not necessary (given our tasks and the random data generation model). In this representation, nodes were represented by squares. We also decided that rows and columns should be distinguishable whatever the number of nodes. We therefore drew the grid of the matrix with lines of width 1 pixel. Finally, row and column size (resp. height and width) has been set as large as possible to maximize space usage.

As we maximized the space usage in the computed images, and due the different natures of the two visualization techniques, nodes in NL appear larger than in AM (see Figure 2).

4.1.4 Deep convolutional network architectures

For this experiment, we have selected two common convolutional networks architectures. On the one hand, we selected a simple yet efficient architecture for solving simple problems. That architecture (see left-side of Figure 3), called LeNet [29], contains 8 layers and has been initially designed to recognize hand-written digits from small 28 × 28 images. On the other hand (see right-side of Figure 3), we selected a much more complex architecture, called VGG16 [43], that has been shown to perform well with complex image classification problems. Haehn et al. [24] mentioned that VGG architecture provides the best results out of their four tested architectures. It seems therefore to be a good candidate to run comparison between visualization techniques. That architecture contains 21 layers and has been initially designed for large scale image classification problems. Table 1 provides the number of parameters to learn for each configuration. Although the VGG16 architecture is more complex than LeNet, its smaller number of parameters is explained by the smaller output of the last pooling operation: 32768 that requires 134221824 weights to learn in the next layer in comparison to a 49152 output with 201330688 weights for LeNet. We have chosen a classification approach instead of regression approach (i.e., the models predict a class instead of a value) in order to generalize them for other tasks in the future. For the same reason, the output layer has also been oversized (i.e. some classes do not appear in the data) in comparison to the number of classes to predict in order to be more dataset independent.

In our experiment, we trained the models (one for each selected architecture) to solve only one out of the three tasks with one visualization technique (NL or AM). Each network has been trained from scratch (as opposed to pre-trained networks) and no weight was shared between the networks of a same architecture for the different tasks (as it could be done by Haleem et al. [24]). Each model has been trained during 100 epochs using negative log likelihood loss and the Adadelta optimizer [48] that has the advantage of requiring no manual tuning of the learning rate.

4.2 Technical details

The generation of graphs and their two representations is done by a tool written in C++. Graph drawing and clustering algorithms respectively used for NL and AM are provided by Tulip framework [5]. Images are then computed from these representations using the ImageMagick library. The models are written in Python with the BigDL [13] library that relies on Keras [12] for the deep learning side and the Apache Spark [47] big data framework for the execution side. The execution platform is composed of 996 cores distributed on 35 datanodes for total of 1.92 TB of RAM and 250 TB of storage.

4.3 Results

We are interested in verifying if we are able to learn the model, how they perform and how they compare between the two graphs representations in order to validate our hypothesis. Another interesting point is the convergence speed of the learning. This section presents these different aspects.

4.3.1 Learning feasibility

As mentioned in Section 3 it is mandatory to determine whether the models were able to learn how to solve the tasks. Even if we use in this experiment classification models, the problem the models have to solve is rather a regression one as the goal is to predict a value (i.e. the number of nodes). We therefore used $R^2$ metric to assess how well the models did learn. Table 2 shows the $R^2$ scores of the best models (selected during the model selection
Table 2: $R^2$ scores of the best models (selected during the model selection step) for each combination of task, network architecture, and visualization technique (1.0 values are due to rounding). These results show that whatever the considered task, network architecture and visualization technique, the models perform better than random choice.

| Task | Network Architecture | AM | NL |
|------|----------------------|----|----|
| Task 0 | LeNet | 1.0 | 0.73 |
|       | VGG16 | 1.0 | 0.97 |
| Task 1 | LeNet | 1.0 | 0.99 |
|       | VGG16 | 1.0 | 1.0 |
| Task 2 | LeNet | 0.98 | 0.97 |
|       | VGG16 | 0.98 | 0.97 |

Figure 4: Confusion matrices with the best model for each task and representation, computed on the test database. LeNet and VGG16 models have been trained for solving the three considered graph visualization tasks on both AM diagram and NL diagram and according to the mse of their predictions. On a perfect performing system, the diagonal is dark blue while the other cells are white. VGG16 seems to perform better than LeNet on NL representation while the opposite can be observed for AM representation.

4.3.2 Models performances and comparison

Table 2 summarizes the classification results using different metrics computed on $V_{test}$ by the models performing the best on $V_{validation}$.

Our hypothesis was that that automatic evaluation should reproduce the results of Ghoniem et al. [19,20], i.e. AM should outperform NL for each of the three tasks. To validate our hypothesis on each task, we selected for each metric (accuracy, percent10, delta10 and mse) the best models (one for each architecture) for each visualization technique. For instance, Figure 4 shows the confusion matrix of the best models selected using mse for each step) for each combination of task, network architecture, and visualization technique. These $R^2$ scores range from 0.73 (for the Task 0 and NL with LeNet architecture) to 1.0. These $R^2$ scores, far from 0, show that both LeNet and VGG16 were able to learn how to solve each of the three tasks with each of the visualization techniques.
Table 3: Summary of the results obtained for each group of task, network and evaluation metric. For each triplet, the best epoch is obtained from the validation database while the presented performance is obtained from the test database. The best configuration over the rows is presented in bold.

| Task | Evaluation | Representation | Performance | Best epoch |
|------|------------|----------------|-------------|------------|
|      |            | Network | AM | NL | AM | NL |
| 0    | accuracy   | LeNet    | 1.0 | 0.1 | 11 | 33 |
|      |            | VGG16    | 1.0 | 0.15 | 18 | 25 |
|      | delta10    | LeNet    | 1.0 | 0.86 | 5  | 47 |
|      |            | VGG16    | 1.0 | 0.97 | 13 | 24 |
|      | mse        | LeNet    | 0.0  | 143.6 | 11 | 47 |
|      |            | VGG16    | 0.0  | 19.23 | 18 | 25 |
|      | percent10  | LeNet    | 1.0  | 0.71 | 5  | 47 |
|      |            | VGG16    | 1.0  | 0.82 | 14 | 24 |
| 1    | accuracy   | LeNet    | 0.95 | 0.19 | 69 | 49 |
|      |            | VGG16    | 0.96 | 0.51 | 86 | 49 |
|      | delta10    | LeNet    | 1.0  | 0.4  | 17 | 76 |
|      |            | VGG16    | 1.0  | 0.29 | 17 | 76 |
|      | mse        | LeNet    | 0.04 | 1327.56 | 17 | 38 |
|      |            | VGG16    | 174.04 | 606.15 | 59 | 55 |
|      | percent10  | LeNet    | 1.0  | 0.61 | 17 | 78 |
|      |            | VGG16    | 0.95 | 0.74 | 86 | 49 |
| 2    | accuracy   | LeNet    | 0.29 | 0.25 | 16 | 15 |
|      |            | VGG16    | 0.28 | 0.26 | 19 | 36 |
|      | delta10    | LeNet    | 1.0  | 1.0  | 7  | 5  |
|      |            | VGG16    | 1.0  | 1.0  | 19 | 6  |
|      | mse        | LeNet    | 2.64 | 4.92 | 10 | 64 |
|      |            | VGG16    | 2.64 | 3.37 | 19 | 31 |
|      | percent10  | LeNet    | 0.66 | 0.56 | 10 | 24 |
|      |            | VGG16    | 0.64 | 0.63 | 19 | 31 |

visualization technique. Then we evaluated how well each model approximates the ground truth by computing for each graph the absolute difference between the ground truth and the model prediction (see Table 4). For each selection criterion (i.e. metrics), we compared these absolute differences for AM and NL. We used the Wilcoxon test that verifies if these two sets of data share the same distribution. If the p-value is lower than 0.05, we can consider that they are different in favor of the one having the smallest median, otherwise no statement can be done. This process is repeated four times by using the best models obtained with the evaluation metrics (mse, accuracy, percent10, delta10). Table 4 shows that the p-value is systematically << 0.05 (so the distributions are different) in favor of the AM representation; Kruskall Wallis test provides the same results. These results validate the hypothesis that AM outperforms NL for the three considered task.

Even if statistical tests validated our hypothesis, we have further analysed the results to identify if one of the dataset generation parameters has an influence on the performances of the models. Figure 3 groups the recognition performance per range of nodes and per density to locally identify the difficult cases on models that minimize the accuracy metric. Concerning Task 0 and Task 1, AM accuracy does not seem affected by neither the number of nodes nor the edge density of the graph. For these tasks, NL accuracy abruptly decreases when graph size exceeds 30 nodes and then remain stable up to 100 nodes. Moreover, NL accuracy also seems to increase with increasing edge density which is surprising. However, the NL accuracies are very low and it may not be relevant to compare them. Concerning Task 2, both NL and AM accuracies decrease when graph size or edge density increase. Such an impact on the accuracy was expected and confirmed the results of Ghoniem et al. [19,20].

4.3.3 Models convergence

Another interesting aspect of such a study is to determine which visualization technique is prone to fast convergence of the model. We think it is correlated to the difficulty of the problem: a fastest convergence means an easier problem and a slowest convergence means a more difficult problem. In our experiment, models trained on the AM representation usually train faster (24 epochs to obtain the best model in average) than models trained with the NL representation (39 epochs in average). The difference is statistically significant as a Wilcoxon signed rank test computed on these 18 pairs obtained a p-value of 0.016 << 0.05. The models therefore learn faster how to solve the tasks with AM representations than with NL representations. Interpreting that learning speed is thorny but we might consider that it would be easier for a user to learn how to solve the tasks with AM representation than with NL representation.
Table 4: Statistical validation of the hypothesis: models trained with AM obtain better performances than models trained with NL. For each task, the mean of the absolute difference between the ground truth and the prediction is shown for AM and NL over all the possibilities graph × representation; the p-value of the Wilcoxon test is also provided (0 values are due to rounding issues).

| Task | Model selection criterion | Mean of abs. diff. AM | Mean of abs. diff. NL | p-value |
|------|-------------------------|----------------------|----------------------|---------|
| Task 0 | mse                     | 0.00                 | 4.64                 | 0.00    |
|       | accuracy                | 0.00                 | 4.86                 | 0.00    |
|       | percent10               | 0.05                 | 4.66                 | 0.00    |
|       | delta10                 | 0.05                 | 4.66                 | 0.00    |
| Task 1 | mse                     | 0.98                 | 20.15                | 0.00    |
|       | accuracy                | 1.00                 | 20.38                | 0.00    |
|       | percent10               | 1.01                 | 19.90                | 0.00    |
|       | delta10                 | 1.01                 | 20.15                | 0.00    |
| Task 2 | mse                     | 1.16                 | 1.46                 | 3.03 × 10⁻⁹ |
|       | accuracy                | 1.17                 | 1.53                 | 9.85 × 10⁻⁶⁰ |
|       | percent10               | 1.16                 | 1.44                 | 8.76 × 10⁻³⁹ |
|       | delta10                 | 1.24                 | 1.66                 | 8.99 × 10⁻⁷⁸ |

Figure 5: accuracy on the test dataset for all the couples of network and representation grouped by range of nodes, and edge densities. The selected models minimize accuracy on the validation dataset.

Figure 6: Ground truths distribution for the 3 tasks in the test database. The distributions are similar for the other two subsets.

4.4 Limitations

As for any evaluation, the results we present in this section can only be interpreted within the limits set by the evaluation protocol. This includes all the parameters of the protocol: the dataset, the algorithms used to generate the layouts, resolution and visual choices for drawing the images, etc.
Our database has been tailored for task 0; Figure 6 presents the ground truth distribution for the 3 tasks on the test database. As expected, the distribution of the number of nodes is nearly uniform (the variation is due to a uniform sampling of the entire dataset). However, the distributions of the number of edges and of the maximum degree clearly do not follow a uniform distribution (but rather a power-law distribution) which also was expected. Indeed, small graphs with high edge densities may have the same number of edges than larger ones with low edge densities. Even if it may have been better to generate datasets especially designed for each task, the purpose of our study was to check whether the results of Ghoniem et al. [19,20] could be reproduced when using our methodology or not. As such unbalanced distributions are due to the dataset generation parameters from [19,20], we could not avoid that bias.

To draw a graph with the NL representation, it is first necessary to compute its layout with a specific algorithm and its particular configuration parameters (Section 4.1.3). The results of the classification, as well as the drawn conclusions, could be different depending on whether it is a non-force-directed algorithm or a force-directed algorithm. We can assume that the CNN models may be more efficient if the graphs were drawn in an orthogonal manner [10]. Similar concerns could be done with the AM where it is known that several encodings can be used to draw the edges [4] and that several node orderings could be used to ease reading [6]. However such limitations are inherent to any evaluation being automatic or human-based and are not specifically related to our methodology.

The last main limitation of our study lies in the image resolution and visual choices for the rendering of the image. Concerning the AM, our rendering engine renders gridline with a constant thickness (1 pixel), increasing the image resolution would increase rows height and columns width, it could also ease the completion of the considered counting tasks. One can have similar concerns about the rendering of NL for which nodes size and edge thickness had to be arbitrarily set. Moreover, to reduce the computational time and memory consumption during the training of the models, we used grayscale as mentioned in Section 4.1.3. This drastically reduces the memory usage and the computational cost as the input image is coded with one channel instead of three in RGB. While colour is usually considered as an important visual channel, we consider it should not penalize the models because the number of colours used is quite small (3) and their grayscale conversion is not ambiguous.

5 Discussion

While it seems that our methodology can reproduce results from the literature, it also suffers from several limitations. We discuss in this section the three main limitations that we have identified.

In most of the formal user evaluations, the user is asked to solve a given task in an interactive environment: in Ghoniem et al. studies [19,20], the user can zoom in/out, pan or even highlight the neighborhood of a given node to ease task completion. On the one hand, providing interaction tools may make the evaluation more realistic as no visualization software would provide only still images. But on the other hand, providing interaction tools may restrict the scope in which the results can be interpreted as the evaluation does not only compare several visualizations but rather compare combinations of visualization and its associated interaction tools. This is particularly true when comparing multiform visualization techniques where the provided interaction tools have to be adapted to each technique. These variations may also induce variations in the results.

The second main limitation of our methodology relates to the relative performances of humans and computer vision techniques. Indeed, we cannot assume that there are nowadays model architectures that can correctly mimic human behaviors including all our imperfections. The performances of a given model for a given task and visualization technique cannot be interpreted as it is since we do not know how these performances are correlated to humans ones. Instead, we make the assumption that if a machine learning model can complete a task more easily with a visualization technique than with another, then the same difference of performances should observable with users. While visualization designers must arbitrarily chose which visualization techniques should be compared, we propose here a methodology that provides a rational argument. Moreover, such an automatic experiment is reproducible and the previous obtained results can serve as baselines for the next visualization techniques.

Last concern of our methodology is related to its computational cost. Performing the proposed evaluation was more difficult than expected. As described in previous section, VGG16 and even LeNet have many parameters to optimize. With the infrastructure described in Section 4.2 and using 48 GB of RAM on each data-node, we could train the models with a batch size of 400 images. For VGG16, training a model (100 epochs) for one task and one visualization took one day and for LeNet, 4 hours. So, training times is not proportional to the number of parameters to train, but rather to the number of operations to execute. With the best settings, we thus computed all our results in one week on our infrastructure. Such a computation time is still a limitation of our methodology, we assume that progress in hardware dedicated for machine learning will enable to run such experiments in less than a day soon.

6 Conclusion

This paper has presented a new methodology for the automatic evaluation of visualization techniques. It makes use of emerging supervised learning methods. Training models to solve a given task with several types of representations and comparing their performances on each of these representations allows to assess their efficiency. Such a comparison cannot replace user evaluations but will serve to properly define/refine hypotheses and/or to explore more thoroughly the design space. Our methodology has been applied on the comparison of two well-known graph visualization techniques: AM and NL diagrams. It confirmed that the machine-learning based results are similar to human-based results. Our experiment proves that models trained with the AM representation learn faster than models trained with NL representation and that models trained with AM representation also perform
better than model trained with NL one. The proposed methodology is validated as similar results were obtained with a human-based evaluation. We therefore believe that it could be applied to other tasks, dataset and visualization techniques.

An interesting direction for future work is to further compare NL and AM diagrams for other tasks from the literature, with other graph properties (e.g. scale-free or small-world), with other graph drawing (for NL diagram) and node ordering algorithms (AM diagram). Another direction could be to include interactive visualization in the methodology. Indeed, the current proposal supports still pictures while user evaluations usually consider interactive visualization. Reinforcement learning [52] seems to be a good option as with such technique an agent could interact with the visualization to learn how to solve a given task.

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