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Deep Dive into Deep Neural Networks with Flows

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Abstract: Deep neural networks are becoming omnipresent in reason of their growing popularity in media and their daily use. However, their global complexity makes them hard to understand which emphasizes their black-box aspect and the lack of confidence given by their potential users. The use of tailored visual and interactive representations is one way to improve their explainability and trustworthy. Inspired by parallel coordinates and Sankey diagrams, this paper proposes a novel visual representation allowing tracing the progressive classification of a trained classification neural network by examining how each evaluation data is being processed by each network's layer. It is thus possible to observe which data classes are quickly recognized, unstable, or lately recognized. Such information provides insights to the user about the model architecture's pertinence and can guide on its improvement. The method has been validated on two classification neural networks inspired from the literature (LeNet5 and VGG16) using two public databases (MNIST and FashionMNIST).

1 INTRODUCTION

There is a growing interest and usage of deep neural networks in various domains (LeCun et al., 2015) during the last decade as they offer reliable assistance in solving problems with good performances. For instance, data classification (Krizhevsky et al., 2012), image segmentation (Delassus and Giot, 2018), data generation (Goodfellow et al., 2014) and reinforcement learning (Mnih et al., 2013) are some tasks expected to be accomplished by such technology.

Deep Neural Networks (DNNs) rely on the composition of simple functions in order to produce a globally complex one that is strongly dependent on factors that are not fixed by the architect when assembling the model layers. When a model processes input data, each neuron computes and returns one value which has a variable impact on the final result. This value also depends on weights fixed during the training phase which itself relies on a dataset given by the trainer. The common question Q1: *How well is the model performing ?* is usually answered with various evaluation metrics, but since the model inner workings are dependent on the architecture, the training dataset and the learning process at once, it is difficult to understand and explain those performances, and neural networks are then of-

ten considered as "black boxes". For this reason, it is difficult to improve or debug models and answer the following questions without proceeding to expensive tries, testing different network architectures and/or parameters in order to verify various hypotheses: Q2: *Should we add or remove layers in the model?* Q3: *Should we change the number of filters of that convolutional layer?* Q4: *Is our training dataset efficient enough to train our model?*

Recently, various works leverage information visualization in order to progress into the field of explainable artificial intelligence. Consequently, several explanation techniques have been presented and implemented with visual interfaces (Hohman et al., 2018) and help to answer similar questions. To design such visual interfaces is a real design challenge because of the complexity of neural networks. For instance, simple typical handwritten digit recognition models (Le-Cun et al., 1998) are commonly composed of at least ten layers, composed themselves of thousands interconnected neurons, involving millions of parameters.

The main contribution of this paper is a novel visualization technique that helps to address the questions Q1, Q2, Q3 and Q4. It relies on studying how data is being processed by a trained model during its evaluation. Using this visualization method, the progressive classification of input data and how each model layer contributes to this task is being revealed. The originality of the method corresponds to:

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Figure 1: Approach overview: First step is to collect information during a network evaluation, then apply an analysis method on it, cluster the results, then render them into a flow visualization.

− its *versatility* by not being specific to the nature of the data being processed by the model (e.g. no constrains to pictures or words);

− its *independence* to the model architecture and inner neuron connections;

− its *compatibility* with any kind of information which is computable at the model layer level such as neuron activation, gradients, analysis methods (such as contribution analysis) or saliency;

The paper is organized as follows. Section 2 presents related works on DNN deep neural network explanation and visualization techniques. Section 3 gives an outline of the proposed method and its inner details in Section 4. Section 5 presents several case studies of the method. Finally, Section 6 discusses on the limitations and future evolution of that work.

2 PREVIOUS WORKS

Explainable machine learning becomes a requirement for legal reasons (Goodman and Flaxman, 2016) and one can leverage on interactive information visualization to achieve this goal. Several methods and tools have already been designed for classification models.

Neuron activation aggregation consists in examining the aggregation of every intermediate result computed by each layer of the model. Using visualization methods such as matrix views, as seen in ActiVis (Kahng et al., 2017), CNNVis (Liu et al., 2016) and in the work of Harley (Harley, 2015), one can find processing similarities between different input data, helping in the understanding of classification patterns. *Forward data projection* is another explaination method using dimensionality reduction and projection techniques (Saeed et al., 2018) to project activation maps into 2-dimensional spaces, allowing the user to obtain an intuitional knowledge about the classification process. This kind of visualization is extensively

used in explaination tools, such as TensorBoard (Abadi et al., 2015), ActiVis (Kahng et al., 2017), Deep-Eyes (Pezzotti et al., 2017) or Re-VACNN (Chung et al., 2016). Analog to data projection, *backward data propagation* aims to explain data transformations by rebuilding the original input data starting from the later layers of the model (Zeiler and Fergus, 2014; Springenberg et al., 2014; Montavon et al., 2018; Montavon et al., 2017). This method is useful in a way that pertinent detected features by the network can be highlighted to the user, which is helpful in the case of image classification (Ribeiro et al., 2016; Olah et al., 2018). Other strategies exist, such as *model comparison* (Zeng et al., 2017; Zhang et al., 2018) which consists in comparing models to detect learning differences.

Several tools emphasize on different data analysis and visualization techniques at once. ActiVis (Kahng et al., 2017) choses to focus on multiple analysis methods for fully connected layers while others tempt to collect as much information as possible on the full network and complete dataset (Liu et al., 2018); some focus on the manner data is being progressively classified using data flow visualizations and techniques previously mentioned. Such systems can be seen in CNNVis (Liu et al., 2016), Summit (Hohman et al., 2020), and some experiments on Distill (Olah et al., 2018), which are focused on image classification, and Neural Network Playground (Smilkov et al., 2016), which proposes an interactive neural network building tool mixing network representation and forward data projection. Those visualization systems give hints on active parts of the model and justify its decision. The method presented in this paper belongs to this category. By combining previously cited analysis methods and presenting their results into a data flow visualization. However, instead of clustering data based on neuron behavior as seen in CNNVis (using mean neuron activation values) or Summit (using top *k* active neurons), this method clusters data based on the similarities of activation maps using an existing analysis method. Displayed flows on the visualization tool can be considered as data being similarly processed, showing the network's progressive dataset classification.

3 APPROACH OVERVIEW

This section presents the set of challenges and requirements that were identified in order to answer questions Q1 to Q4. Figure 1 depicts the complete step-by-step process going from the collection of data related to the evaluation of a model to its visualization.

A network is composed of connected layers that act as a succession of data transformations from the input to the output. Each layer transforms its input data in values and shape before feeding it to the next layer. Those intermediate values are called "activation maps" and are usually seen as multidimensional matrices. It must be noted that activation maps usually reach high levels of dimensionality (e.g. VGG16's activation maps reach sizes of $28 \times 28 \times 256$ shaped matrices) and can be technically challenging to handle by a classic computer: (R1): The method must scale to gigabytes of data computing.

The chosen analysis method makes use of all of the activation maps computed for each input sample. Furthermore, to compare good model prediction from bad model prediction, (R2): Each activation map must be collected in order to support layered highdimensional data analysis, along with its ground truth and its model prediction result.

The visualization method must be a reliable tool to answer Q1 to Q4. Q1 is usually expressed with a metric such as accuracy and/or loss function. This metric is easily interpretable by the user, and (R3): The recognition performances must be limpidly reflected on the visualization.

The classification performances of a model are usually related to the quality of the refinement process across its layers: early layers detect low-level features (e.g. shapes in pictures) and later layers build correlations between those features. To help answer questions Q2 to Q4 and by following this concept, (R4) The refinement process must be noticeable on the visualization.

Finally, in order to debug the model, the method gives more precise answers to Q2 and Q3 by presenting how the refinement process is evolving across the network. To compare each layer refinement performance with others gives insight on where the model needs improvements, and this comparison can be achieved using analysis method as mentioned in the previous section and must be encoded in the visualiza-

tion: (R5) Each layer contribution to the classification process must be comparable with others.

To address R1 and R2, one can leverage large scale computing infrastructure such as computer clusters. Modern systems are able to handle petabytes of data at reasonable cost, which is appropriate to analyze complex networks, as computation charge can be distributed since the evaluation of a single input sample does not require information from other samples.

Processing large quantities of high-dimensional data implies a proper perceptual scalability: in the case of R2, it is frequent to visualize computed data into a 2 dimensional space using various linear (e.g. PCA) and nonlinear (e.g. t-SNE) data projection methods. To efficiently interpret the results of the analysis method, clusters are being built, for each layer L^I , as follows: given L_x^I the activation map computed by L^I for the input data *x* and *f* the chosen analysis function, the input data *a* and *b* are in the same cluster if, and only if $f(L^I_a) \sim f(L^I_b)$.

Addressing $R3$ is done by evaluating the cluster compositions computed on the model's last layer: a perfect classification implies each element of a same cluster has the same ground truth as the others, while a bad classification will lead to more heterogeneous ground truth among the elements of a same cluster.

Following the clustering approach, addressing R4 and R5 is related to the visualization of evolving cluster compositions over layer traversal. That topic has already been studied previously to represent a storyline (Tanahashi et al., 2015) or to visualize the evolution of software components (Telea and Auber, 2008). Design choices are mainly based on these previous results. Clusters of each layer are represented using a containment diagram, composed of their respective input data. Since the method is considering a large amount of input data, it was a design choice not to represent them individually. Instead, each cluster is sized proportionally to its cardinality, then segmented proportionally for each ground truth present in its composition. This approach enables to meet R3 and R5, but R4 is trickier to address. To trace each input data during the refinement process, the same metaphor as a storyline has been used: mainly inspired by parallel coordinates diagram, it consists in drawing connections between clusters of consecutive layers which contain a same set of input data.

4 APPROACH DETAILS

This section details each step of the method proposed in this paper. The overall process can be split into two parts: a first procedure which focuses on col-

Figure 2: Visualization result on a LeNet5-inspired model evaluated on MNIST.

lecting data, applying analysis method and clustering results, while the second procedure transforms those results into a flow visualization.

4.1 Implementation choices

In order to evaluate a layer's performances, activation maps analysis is not sufficient; how each individual neuron value is impacting on the rest of the neural network is also important. The Layer-wise Relevance Propagation analysis method (Montavon et al., 2018), or LRP, is a method measuring each neuron contribution to the rest of the computation. This is done by the propagation of the model's final activation maps back to the input space by estimating each layer contribution thanks to the weights of each neuron. This method was chosen to detect the different contribution patterns a layer could bring to the rest of the network. By comparing each pattern with others and labeling their respective data classes, it allows to measure which input data was finely processed by the layer and which were not. It should be noted that the LRP analysis function is not tied to the proposed framework and other analysis methods can be applied if needed.

Each pattern is represented as a node of a graph and its similarity measure with others as weighted edges. With that, the Markov Cluster Algorithm (Dongen, 2000), or MCL, can be applied on the graph to generate clusters of similar patterns. This algorithm is an efficient scalable method to find dense communities of nodes in a graph by simulating a random walk on it, which is influenced by the edge weights.

Algorithm 1 Data collection and processing

procedure PREPAREDATA(*M*,*D*, *f*) % *M*: a DNN to inspect % *D*: an evaluation dataset $%$ *f* : an analysis function % *act*,*res*, *pred*,*C*: empty associative lists for all $x \in D$ do $act[x] \leftarrow getActivational(\textit{A} x)$ $res[x] \leftarrow applyAnalysis(f, act[x], m)$ $pred[x] \leftarrow getModel Prediction(m, x)$ end for

```
for all L^I \in M.layers do
         V \leftarrow \forall x \in D : res[x][L^I]M \leftarrow \text{buildSimilarityMatrix}(V)M' \leftarrow applyKNN(M, k)C[l] \leftarrow applyMCL(M')end for
    return (C, pred)
end procedure
```
4.2 Data analysis and clustering

Algorithm 1 depicts the procedure which is expensive to compute. As mentioned earlier by addressing R1 and R2, it should be processed using distributed computing on a computer cluster.

As it can be seen, the procedure is performing two iterations: the first one over the evaluation dataset to collect and perform analysis over model computations, the other on each layer to prepare those results into specific encodings. They can be efficiently performed across computer clusters, since neither iterations is

depending on their previous state.

getActivationMaps (R1): The first step is to collect the data transformations of each model's layers for the current input data. This collection may be done by various ways, but it is necessary to keep a record of which activation map belongs to which layer.

applyAnalysis (R2): The chosen analysis method is being applied. This algorithm will transform activation map values while keeping the multidimentional aspect of the matrices.

getModelPrediction (R3): The model predictions are collected to label data flows during the visualization encoding.

buildSimilarityMatrix (R3, R4): In order to cluster the data, it is necessary to first vectorize each element of the evaluation dataset into their *n*-dimensional space imposed by each layer of the model. For example, a matrix *M* of size $16 \times 16 \times 64$ resulting of a convolutional layer will be vectorized into *V* as: $V = [M_{1,1,1}, M_{1,1,2},...,M_{1,1,64}, M_{1,2,1},...,M_{16,16,64}]^T.$ Those vectors can be compared to each other using a similarity metric. Measuring similarity of one vector against each other builds up a similarity matrix which will be used to cluster data. Cosine similarity was used in the scenario of the section 5 to emphasize on pattern diversity rather than neuron value magnitude computed by Euclidean similarity. The construction of these similarity matrices is an extremely expensive operation because of the amount of comparison to perform $(O(n^2))$ and the compared vector size.

applyKNN (R3, R4): The previously built similarity matrix corresponds to a graph of weighted edges. However, this graph is very dense because the similarity between all the elements has been computed. To obtain a sparser graph which is adequate to cluster, one can filter out some edges with low weight.

However, removing edges lower than an ε factor does not guarantees that the graph is still connected and may overly bias the clustering algorithm leading to misinterpretation of the clusters, as each node being left out will form a cluster by itself. Instead, a KNN approach is presented, which will filter out low weighted edges from dense communities, while keeping the connexity of the graph. As for the *k* factor of the KNN algorithm, it was arbitrary considered that a pattern could not be similar to more than *D*/*N* other samples, *D* being the dataset size and *N* the number of different classes present in the evaluation dataset. The edges filtered out by KNN were set at a weight of 0.

applyMCL (R3, R4, R5): The final operation is to cluster the graph in order to obtain a list of clusters and their composition. Along with the prediction data computed earlier and the evaluation dataset, there is enough information to trace how the evaluation data

was processed by the model. The size of this information is also significantly lower than the analysis method computation and the similarity matrices, while keeping the essential information.

4.3 Visualization generation

Algorithm 2 presents the visual encoding process. Compared to the first procedure, this one is way less expensive to compute, mainly because of the data size to process, and can be performed on a single, classic computer.

generateClusters (R3): To display the overall predictions versus ground truths in the same way as the layer contributions to the classification, clusters of input data are artificially built based on their model prediction and their ground truth. This approach is used to compare the visualization results with actual performances of the model, and is discussed in the next section.

buildDAG (R3, R4): Similarly to the parallel coordinate visualization method, this visualization can be represented as a directed acyclic graph, or DAG; each cluster will be represented as a vertex, and each edge will signify that there is a same single sample in the two concerned clusters. A constraint is applied on the vertex coordinates (x, y) , in which *x* will be related to the cluster's layer position in the model, and *y* will be different for each cluster of a same layer, in order to not overlap each other.

orderDAGVertices (R4): Before drawing the DAG, its readability can be improved by reducing edge crossing by ordering each vertex along its *y* coordinate. Here, the barycentric ordering, described in the work of Sugiyama (Sugiyama et al., 1981), is applied mainly because of its ease of implementation and efficiency.

mergeEdgesIntoFlows (R4, R5): The diagram's flows must represent a quantity of data that shares similar information. Here, the information displayed is the ground truth of the concerned samples and the connected clusters. Edges of input data that share the same ground truth and extremities are thus merged together. The merging result is a DAG with the same vertices as before, but with weighted edges reflecting the ground truth of the data they represent.

drawFlows (R3, R4, R5): The computed data is now a graph in which each vertex describes a cluster, its composition, and its position in the visualization, and each edge describes a flow, its starting position and destination, and its composition, in which each item shares the same ground truth.

In continuation of what was addressed for R4 and R5, a color is assigned to each ground truth, and clusters are represented by "boxes" which are colored in a way to indicate the proportion of each ground truth into their compositions. Flows are represented as colored transparent Bezier curves to ease their reading. Furthermore, each axis is labeled by the type of layer responsible for the clustering, and a legend is being added to understand how each data classes are being represented.

5 CASE STUDIES

This section sets out several realistic use cases to validate the method. They rely on two distinct convolutional neural networks for classification:

− A simple model inspired from LeNet5 (LeCun et al., 1998) which is a fairly popular, simple and efficient model designed to recognize handwritten digits. It serves as an example to illustrate the proposed method.

− An adapted version of VGG16 (Simonyan and Zisserman, 2014) to work on 32×32 pictures. It is more complex and has been designed to classify the ImageNet dataset with high accuracy (Krizhevsky et al., 2012), which is featuring thousands of different classes out of 14 million pictures. Since training such a model has a high computational cost (Simonyan and Zisserman, 2014), convolutional layers of the original model were resized to work with the MNIST dataset while keeping the training results of ImageNet (ie. neuron weights).

Model training and evaluation were done on TensorFlow (Abadi et al., 2015) on an nVidia GeForce GTX 1080Ti using the Keras API (Chollet et al., 2015). The computer cluster is composed of 51 machines for a total of 2.7TB RAM, using Hadoop for data transfers and Spark for task distribution, without optimizations such as efficient memory and computing resources management. The clustering process uses the MCL program proposed by its creator (Dongen, 2000). Finally, the visualization process is implemented as a Web application using the HTML Canvas API. A demonstration of this interface can be found at http://pivert.labri.fr. Table 1 summarizes the performance results of the various scenarios experimented.

Scenario 1: LeNet5 trained and evaluated on MNIST. This illustrative scenario aims to explain how this visualization method helps to understand inner work of a classification model and to determine which classes of the dataset are easier to classify than others. The model was trained (60000 samples) and evaluated (10000 samples) on MNIST during 6 epochs, achieving an accuracy score of 98.5%.

Figure 2 depicts the model classification results. Few divergent flows exist between the Prediction and GT (Ground Truth) axis revealing a few classification errors, but otherwise the classification looks great: the model performances are well represented. The cluster composition between the latest layer (Dense 10) and the Prediction axis are different and will be discussed later. The classification progress across the model is easily distinguishable: some classes are detected early (*e.g.*, 1 and 7) while similar digits are detected later with the help of the second convolutional layer (*e.g.* 0 and 6) or the first dense layer (*e.g.* 4 and 9). A majority of classes are distinguished from each other at the Dense 128 layer, except for a few 5 mixed with 3, and 9 with 4. By looking at the previous layer, it can be seen that the convolutional layer is incorrectly splitting those items leading the Dense 128 into errors.

Scenario 2 : LeNet5 and Fashion-MNIST. The same experiment has been run using the Fashion-MNIST (Xiao et al., 2017) dataset. It is a proposed as an alternative to the classic MNIST dataset, featuring clothing pictures instead of handwritten digits; they share the same input and output shapes and number of classes in order to be interchangeable and is supposed to be more complex. The model was trained with 60000 samples and evaluated with 10000 samples, and reached an accuracy score of 87.9%. Results are not shown due to space issues but are available online. They prove the system works by giving a result similar to the previous scenario with more mixed clusters toward the end of the model. Looking at the convolutional layers shows that data was less sparse before reaching the Dense layers.

Scenario 3 : Detection of bad model - LeNet5 model trained with MNIST and evaluated on Fashion-MNIST. The model was trained to achieve high accuracy on MNIST and is expected to fail on Fashion-MNIST because of the different nature of the processed data. In this case, we use the visualization

Figure 3: Visualization result on a model that has not learned to classify the evaluation dataset.

results to analyze the behavior of the proposed method in a worst case scenario (5.6% accuracy). Figure 3 depicts the visualization result; if differs greatly from the others by the number of clusters generated and drawn. Furthermore, processed data doesn't seem to be equally distributed across computed clusters despite the balanced composition of the training dataset. When looking at the convolutional layers, it seems that a few visual traits have been identified by the model, but wrongly associated with the classes in the later Dense layers.

Scenario 4 : Simplification direction for complex models - VGG16 with MNIST. To adapt the model to the MNIST dataset, we applied some modifications on both VGG16 and the MNIST dataset: (i) MNIST images are considered to be colored image by duplicating the gray channel, (ii) MNIST images are padded to use a shape of $32 \times 32 \times 3$ in order to avoid issues with the latest pooling operation of VGG16 (pooling area larger than the input tensor), (iii) end of the network has been modified to classify 10 classes instead of 1000, (iv) only this latest layer is trained, while the weights of the other layers are transferred from public ImageNet training.

These steps do not replace a full training process of VGG16 on the MNIST dataset, but it still gives us an accurate enough model with an accuracy score of \approx 97%. Since VGG16 is more complex than the previous model, we assume there are unnecessary computations in the model to achieve similar accuracy results. With this experimentation, we expect to see early merged data fluxes in our visualization, meaning that the data is being overprocessed since the activation maps are already similar enough to be predicted as a same class. Figure 4 presents the results. The higher number

of axis displayed is justified by the model's higher complexity. Using transfer learning, although those layers have been trained on ImageNet, the first convolution layers have nicely discerned a majority of classes except of the 5/3, 4/9 and 0/6 couples, which is a behavior really similar to LeNet5. The classification then get stagnant with both improvements and regressions at each pooling operation. By the first Dense layer, most classes are recognized, but there are mixed clusters in the Dense 10 layer, which still provides correct predictions. A few hypotheses can be made: (a) The sudden increase in clustering quality on the first Dense layer means that some of the previous convolution/pooling layers are not very effective in this task. (b) The numerous differences between the Dense 10 and Prediction axis mean that a few classes were in a very similar state by the end of the model. The model still managed to make the right decision, but without high certitude because of the way the Softmax activation works by taking the highest certitude value.

6 DISCUSSION AND **CONCLUSION**

DNNs suffer from lack of explainability and visualization is one way to overcome this issue. This paper has presented a novel way to provide insights on how data are considered by the various layers of a trained network. It helps to answer questions model designers, trainers and non-experts might ask to understand or

Figure 4: Visualization result on evaluating the modified VGG16 model with MNIST dataset. Table 1: Performances overview on each scenario.

improve their model and reduce its "black box" aspect.

The combination of analysis on neuron activation maps and clustering on evaluation data builds up a flexible framework for a simple visualization method. The user can, in one glance, see how data is handled by each layer and understand where sources of misclassifications are, leading to improvements for both the model and the training set.

Being an early prototype, this visualization method can be further expanded and improved, notably in both visualization and clustering quality. As the current visualization system gives good hints on the inner working of a model, experts may need to access more low-level and detailed information about the classification. Usage of distributed computing infrastructure is not a long-term solution to $R1$ and $R2$ when using distance matrix computation, since its complexity is quadratic and thus will be an issue when processing very large evaluation datasets and/or models. Concerning clustering quality, the method used in the previous scenario, namely cosine similarity, presents a few unsatisfactory clustering results, such as the difference between the decision layer's clusters and the actual predictions made by the model. An extensive study on combining similarity and cluster computing method would surely improve the method results. The current flow encoding is limited by the color palette and could lose in efficiency in the case of complex classification networks recognizing numerous classes. Also, layers of complex networks may not be ordered sequentially but instead be composed of multiple branches and junctions, which is currently not supported by such a visualization. Finally, it would be interesting to eval-

uate the usefulness of this method when used during the learning phase of a model, precisely on its capacity at detecting learning specific issues such as overfitting or slow learning rate.

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