Conceptual Content in Deep Convolutional Neural Networks: An analysis into multi-faceted properties of neurons

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Abstract

In this paper we analyze convolutional layers of VGG16 model pre-trained on ILSVRC2012. We based our analysis on the responses of neurons to the images of all classes in ImageNet database. In our analysis, we first propose a visualization method to illustrate the learned content of each neuron. Next, we investigate single and multi-faceted neurons based on the diversity of neurons responses to different classes. Finally, we compute the neuronal similarity at each layer and make a comparison between them. Our results demonstrate that the neurons in lower layers exhibit a multi-faceted behavior, whereas the majority of neurons in higher layers comprise single-faceted property and tend to respond to a smaller number of classes.

Keywords: Deep Neural Network, Deep Visualization, Multi-faceted and Single-faceted Neurons

1 Introduction

The non-linear deep learning approach has achieved a tremendous success in various applications and has revolutionized the area of machine learning and computer vision in recent years. In particular, convolutional neural networks have demonstrated a high flexibility as well as efficiency that can be utilized for a wide range of problems in different domains. In spite of the increasing effort in designing new deep network architectures, still not much is known about the internal representation of these networks and the trained units of deep neural networks are not readily interpretable. Lately, two principle directions for understanding deep neural networks that has been followed are network analysis and network visualization. Several authors have attempted analyzing DNNs using information theory principles to study deep representation. In this regard, (Shwartz-Ziv & Tishby, 2017) (Tishby & Zaslavsky, 2015) viewed DNN as a Markovian compression procedure between input and output of the network and calculated the information bottleneck bound on each layer. In a follow-up research, (Achille & Soatto, 2017) worked on the minimal deep representation. Other researchers have focused on the problem of deep network visualization in order to gain an understanding about the underlying learning structure of these networks. Deep network understanding approaches can be divided into two broad categories of macroscopic and microscopic viewpoints. In the first category, the primary interest is centered on understanding the functionality of deep neural networks as a classification tool and the related questions pivot around the effect of each pixel or region on the performance of the fully connected layers of network in making discrimination between classes. In contrast, the second category seeks to inspect the building blocks of pre-trained deep networks such as neurons and weights.

Regarding the former view, Simonyan et al., conducted a sensitivity analysis and created a saliency map based on the influence of input image pixels on the classification decision(Simonyan & Zisserman, 2014). In a similar vein, Zintgraf et al., studied the effect of each patch that contains a specific pixel(Zintgraf, Cohen, & Welling, 2016). Zhou et al., derived a minimal representation of input images by removing the regions that generated the least decrement in correct classification rate (Zhou, Lapedriza, Xiao, Torralba, & Oliva, 2014)(Zhou, Khosla, Lapedriza, Oliva, & Torralba, 2014).
On the latter view, activation maximization was the target of several researchers. In a number of visualization studies, authors attended to the maximum activation values in convolutional and pooling layers and retrieved the corresponding input patterns or patches (Girshick, Donahue, Darrell, & Malik, 2014) (Erhan, Bengio, Courville, & Vincent, 2009). Yosinsky et al., applied a regularization technique in order to find images that can cause highest activation values (Yosinski, Clune, Nguyen, Fuchs, & Lipson, 2015). Zeiler and Fergus introduced the idea of deconvolution in which they employed reverse computation from activation maps to the input patterns to obtain a heat map that visualizes the most effective area of image that is remarkable in provoking a neuron to fire (Zeiler & Fergus, 2014).

One intriguing property that has been discovered about neurons is that they can respond to various images from different classes. These types of neurons which are called multi-faceted neurons have been found in mediotemporal lobe of the brain and have reported to be activated by pictures of multiple objects (Quiroga, Reddy, Kreiman, Koch, & Fried, 2005). In the realm of deep visualization, a few efforts have been made. Nguyen et al., focused on the problem of multi-faceted visualization (MFV) (Nguyen, Yosinski, & Clune, 2016). They used an optimization algorithm to produce images that maximally activates each neuron. In order to create multi-faceted visualization, they used different initialization images obtained from cluster of images from each class.

Along the same lines with the recent findings in deep network interpretation, we conduct a number of statistical analysis with the purpose of scrutinizing the trained neurons and uncovering the progressive patterns of learning in the deep learning pipeline. We hypothesize that the association between neurons and the class of images that has activated them encompasses conceptual information about the deep representation. In particular, our line of work is concerned with multi-faceted properties of neurons in terms of quantification of the degree of neurons’ responses to different classes as well as a neuron visualization method which relies on finding the independent components of the top images that activate each neuron. Moreover, we investigate conceptual similarity between neurons across deep convolutional layers. In the following sections, we first describe the basic encoding for the neuron and class association. Next, we propose a method for visualization of content of neurons. We describe multi-faceted and single-faceted neurons and our approach for these types of neuron identification in section C. In the final section, we calculate the Euclidean distance and correlation based on our association encoding.

2 Method
2.1 Conceptual encoding
We conduct our analysis based on the vgg16 network pre-trained on ImageNet2012 dataset which contains 1.3 million images from 1000 classes. This network includes five blocks of convolutional layers. Table 1 shows the details of the vgg16 architecture in the convolutional layers. In this paper, we may also refer to the deep layers in a consecutive manner. For example, layer 3 points to the second convolutional layer in block 2.

Table 1. VGG16 net architecture

| Block No. | 1 | 2 | 3 | 4 | 5 |
|-----------|---|---|---|---|---|
| # Conv layers | 2 | 2 | 3 | 3 | 3 |
| # Neurons | 64 | 128 | 256 | 512 | 512 |

As mentioned before, we aim to probe the learned concepts by neurons at each convolutional layer of vgg16 model and study how the conceptual content of neurons develops across deep convolutional layers. In order to capture the association between neurons activations and the corresponding triggered classes
we take the following approach. We encode the conceptual content of each layer based on the appeared classes in the top 100 images with the highest amount of activation values (Girshick et al., 2014) (Rafegas, Vanrell, & Alexandre, 2017). For this purpose, we define a neuron-by-class co-occurrence matrix that measures the frequency of highly activated images. We call this matrix as CoF matrix and refer to each row of it as a neuron vector. Hence, each cell of CoF(n,c) shows the number of images that belongs to class c and has highly provoked neuron n.

2.2 Neuron visualization
In this section we aim to introduce a method for visualization of the information content of neurons at each layer. In essence, we are interested to extract the basis patterns in the 100-top patches of input images that has highly activated neurons at each layer in order to gain an understanding about the basic visual features that has activated each neuron (Rafegas et al., 2017). In addition, the underlying basis of top images yields an insight about the multi-faceted effect of neurons. Past research on neuron visualization has been mainly focused on providing one image for each neuron. We promote the hypothesis that in order to find a detailed explanation of the visualized content of neurons, more than one image is beneficial. Following this idea, we assume that there are multiple sources of information that stimulates each neuron and we seek to find them by applying Independent component analysis (ICA). ICA is a powerful tool that can provide high order representation of images and has been shown to be suitable for the problem of blind source separation (Hyvärinen, Karhunen, & Oja, 2001). It can also be regarded as a dimension reduction technique which can find the original sources of signals. It has been shown that ICA behavior is similar to simple cells in the brain. In essence, the ICA bases structure has shown to resemble the receptive fields of simple cells in primary cortex (Caywood, Willmore, & Tolhurst, 2004).

We applied Independent Component analysis to the list of patches pertaining to each neuron and then visualized the ICA bases or independent components (ICs). ICA is an unsupervised algorithm but the number of components needs to be determined in advance. We tried different numbers and decided to compute eight ICA basis for each set of 100 top patch list of each neuron. The basic components provide visual information about the nature of the images preferred by each neuron. Independent component visualization can reveal the multi-responsive feature of neurons based on the similarity of the patterns captured by each component. If all the components look alike it signifies that a neuron is a single-faceted neuron, otherwise it can be considered as a multi-faceted neuron. We discuss this notion in the next section.

2.3 Multi-faceted vs. Single-Faceted Neurons
Single-faceted(SF) neurons are referred to those neurons in human MTL with selective responses to a single concept (Quiroga et al., 2005). We identify SF neurons as those neurons which highly respond to a particular class of images. These types of neurons are also known as concept neurons or grandmother cells. On the other hand, multi-faceted(MF) neurons are considered as the neurons which are activated by images from range of different classes. We identify SF neurons as those neurons which highly respond to a particular class of images. These types of neurons are also known as concept neurons or grandmother cells. On the other hand, multi-faceted(MF) neurons are considered as the neurons which are activated by images from range of different classes. In order to assess neurons’ conceptual properties, we compare neurons’ responses to classes based on their representations through the rows of CoF matrix. For this purpose, we leverage two measurements: vector sparsity and signal flatness. We calculate the sparseness of each neuron in one layer based on the number of classes from top scoring image list that triggers a neuron, i.e., the sparseness of rows of CoF matrix. We use Gini index in order to assess the sparseness degree (Zonoobi, Kassim, &
Venkatesh, 2011). We chose this coefficient because of a number of advantages that it has over other indexes. It produces normalized values in the range of (0,1) and the values are not dependent on the size of the input vector. The sparsity index captures the frequency of responses of a neuron to multiple classes. Low values of this index is an indication of multi-faceted neurons.

Moreover, we measured the flatness of each neuron. As mentioned before, each row of CoF declares the number of classes that each neuron was triggered by. In other words, each row is a signal which encodes the activation behavior of each neuron. In order to evaluate the flatness of neurons we evaluated the spectral flatness using equations (1) to quantify how much each neuron is oriented towards a concept(Madhu, 2009).

$$\hat{n}_r^l = \frac{n_r^l}{\sum_{i=0}^{N_l-1} n_r^l(i)}$$

$$\log_2 (\text{Flatness}(n_r^l) + 1) = -\frac{1}{\log_2(N_l)} \sum_i \hat{n}_r^l(i) \log_2 (\hat{n}_r^l(i))$$

Where $n_r^l$ is the row $r$ of CoF matrix at layer $l$ and $N_l$ is the number of neurons in layer $l$. In order to prevent the undesired effect of zeros in measurement we first add a small constant of 0.0000001 to all the elements of $n_r^l$. The flatness values ranges between 0 and 1. We decided to attribute the value of -1 for flatness in extreme cases that all the elements of a vector are zero. This is due to the fact that all-zero vectors reflect no response and so cannot be considered as valid cases.

Lower values of sparsity and higher values of flatness is an indication of multi-faceted neurons. We normalized both values and plotted the density of these two values over all neurons in each layer of vgg16 net in Figure 1. In addition, we show the Normal distribution of each of these values at each layer in Appendix A.

![Figure 1. Estimated Normal distribution of sparsity and flatness measurements corresponding to all of the neurons at each layer of vgg16 net.](image)

It is outlined in Figure 1 that as we go across higher layers, sparsity increases whereas flatness decreases. This implies that neurons in higher layers are tended to operate like concept neurons.

We call the multi-faceted capacity of a neuron $n_i$ as MF degree and we define it using equation (2).

$$MF(n_i) = \frac{\text{flatness}(n_i)}{\text{sparsity}(n_i)}$$

Figure 2. illustrates the normalized MF values for all neurons across all layers. We can observe that while the MF degree of neurons in lower layers are higher, it drops as we approach towards higher layers. It is worthwhile to note that while there are too many neurons with high MF degrees, the values are not significantly high. More importantly, we should note that the max value of un-normalized MF degree is 0.63, and the mean value is 0.53.
Moreover, we arranged examples of visualization of one of the four-top neurons based on MF degrees according to our proposed method in Tables 2 and 3. For each value, we have specified the corresponding p-value based on the distribution of all other MF values within the same layer. We consider 0.05 as the cutoff for significance. We interpret neurons MF degrees above mean as a sign of multi-faceted attribute and neurons with MF degrees below mean as single-faceted or concept neurons. For each neuron, ICs are visualized in three different ways. The first column from left shows the ICs in gray scale. The second and third column presents the case in which the ICs are computed individually for each R, G, and B channels and then the channels are combined into a three-dimensional array. The last column exhibits the corresponding converted results in 8-bit unsigned integer. In another attempt, we concatenated all the channels first and then computed ICs but since the results were not semantically comprehensible we decided not to report them. From the results, we can observe that the neurons with high MF degrees tend to have a blurred visualization and their corresponding ICs are dissimilar. In contrast, the visualization of the neurons with low MF degrees incorporate clearer shapes. Figure 4 shows examples of gray-scale visualization of MF and SF neurons that we selected in a qualitative manner along with their corresponding patches. It can be observed that ICs can visualize neurons that respond to different concepts. In blocks 3 and 4 we can also observe meaningful images and distinguish the category of objects. High MF degree indicates that a neuron is activated by patches of images from different classes. But it doesn’t necessarily imply that the pattern of patches should be notably different. We found that although generally, the neurons with high flatness degrees include ICs with different shapes and patterns, this does not apply for all the neurons, esp. neurons in the shallower layers. Furthermore, while most of the highest MF degrees do not yield significant values, the lowest ones do. This puts forward that unlike concept neurons, multi-faceted properties cannot be found too often in shallower convolutional layers. Furthermore, we depict the MF degree corresponding to top MF and SF neuron at each layer in Figure 3. We also show the number of MF and SF neurons scaled by the total number of neurons at each layer in the same Figure. The results are quite remarkable in providing the support that the number of SF neurons grows across the deep layers. In contrast, the number of MF neurons presents a declining pattern. Besides, while the MF degrees of concept neurons keeps decreasing through the deep layers, it is quite fixed for MF neurons.
Figure 3. Number of multi-faceted(MF) and single-faceted(SF) neurons and their corresponding MF degree at each deep layer

Table 2. Single-faceted neurons

| Layer name       | Neuron number | Multi-faceted degree | pvalue within the layer |
|------------------|---------------|----------------------|-------------------------|
| Block 2 – conv 1 | 25 (2nd top)  | 0.49                 | 1.47e-7                 |
| Block 3 – conv 2 | 484 (4th top) | 0.55                 | 0.0006                  |
| Block 3 – conv 3 | 91 (2nd top)  | 0.36                 | 5.8e-5                  |
| Block 4 – conv 1 | 89 (4th top)  | 0.32                 | 0.003                   |
Table 3. Multi-faceted Neurons

| Layer name          | Neuron number | Multi-faceted degree | Pvalue within the layer |
|---------------------|---------------|----------------------|-------------------------|
| Block 0 – conv 1    | 16 (2nd top)  | 0.97                 | 0.01                    |
| Block 0 – conv 2    | 29 (1st top)  | 0.97                 | 0.14                    |
| Block 1 – conv 1    | 91 (2nd top)  | 0.98                 | 0.14                    |
| Block 1 – conv 2    | 85 (1st top)  | 1.0                  | 0.1                     |

**SF Neurons**
Layer 7 – neuron 7

**MF Neurons**
Layer 7- neuron 291
Layer 10-neuron 185

Layer 10-neuron 28

Layer 11-neuron 58

Layer 11-neuron 215
2.4 Neuronal similarity/dissimilarity matrices

In this section, we aim to measure the degree of pairwise neuronal similarity using our aforementioned conceptual encoding. Generally, neuronal similarity can be measured from different viewpoints. Neuroscientists tend to categorize neurons based on their morphological similarities. In this regard, they study neurons’ shape, structure and connectivity (Stepanyants & Chklovskii, 2005)(Kong, Fish, Rockhill, & Masland, 2005). There has also been some efforts in finding the association between morphology and functionality of neurons (Stiefel & Sejnowski, 2007). In this work, we aim to investigate the similarity between trained neurons based on their response to images from different classes. To this aim, we construct neurons similarity/dissimilarity matrices between all pairs of the CoF rows at each
convolutional layer. We use the Pearson correlation to measure the similarity and Euclidean distance to assess the dissimilarity between each pair of neurons in each layer. RDM and RSA of CoF matrices are provided in Appendix A. Figure 5 presents the average conceptual similarity and dissimilarity of CoF matrices at each layer.

![Figure 5](image)

The results show that average conceptual similarities decrease as we pass over deeper layers. In other words, neurons become less correlated and more specialized in the higher layers, while neuronal dissimilarities exhibit a more incremental progression. This can be explained by the fact that in the lower layers, neurons act as low feature detectors whereas neurons in the higher layers serve as shape-like detectors and so are more disposed to be less correlated. More importantly, the similarity matrices can also be viewed as a way of capturing the multi-faceted property. Higher similarities can be interpreted as a sign of multi class preferences. In contrary, low similarities highlight the existence of singular neurons that account for particular concepts. This interpretation is also compatible with our finding in the previous section that the distribution of concept and multi-faceted neurons are not equal in all layers and it drops towards higher layers.

### 3 Discussion

To recap, in this work we studied neurons conceptual content in VGG16 pre-trained on ImageNet2012 Competition data. To this end, we created a co-occurrence matrix that counts the classes that each neuron responds to. We further identified concept and multi-faceted neurons by measuring the sparsity and flatness of each row of the co-occurrence matrix and then calculated the multi-faceted degree of each neuron. Moreover, we proposed to use ICA technique as an approach for neuron visualization. The upside of taking this approach is that it can provide different aspects of learned content of each neuron using a set of images. To our knowledge, this is the first study that puts forward the idea of using a set of images for reflecting underlying learnt content of neurons in a deep network. The ICs corresponding to a SF neuron are expected to include similar patterns and visualize more coherent shapes of specific concepts. Finally, we computed the Neuronal similarities in each convolutional layer on the basis of their classes response reaction. This experiment helps to gain an understanding about neurons’ pairwise functional similarity. In our experiments we demonstrate the unequal distribution of MF and SF neurons across deep layers. In essence, our results suggest that neurons that are lied in lower convolutional layers mirror less preference in responding to different classes, while neurons in the higher deep layers can be activated by a range of multiple classes.
Appendix A) Distribution of sparsity and flatness values of population of neurons in each layer

A1. Distribution of flatness of neuron in layers of vgg16 network
A2. Distribution of sparsity of neurons in layers of vgg16 network
Appendix B) Additional visualization based on numerical values

a)  
| Layer number | Filter number | MF degree | Neuron type |
|--------------|---------------|-----------|-------------|
| 0            | 12            | 0.91      | MF          |
Appendix C) heat maps of similarity/dissimilarity matrices

a) conceptual dissimilarity measured by Euclidean distance on CoF matrix- from right to left and up to down, convolutional layer 1 to convolutional layer 13
Layer 10

Layer 11

Layer 12

Layer 13

b) conceptual similarity measured by Pearson correlation on CoF matrix - from right to left and up to down, convolutional layer 1 to convolutional layer 13
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