Explaining Representation by Mutual Information

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Abstract

Science is used to discover the law of world. Machine learning can be used to discover the law of data. In recent years, there are more and more research about interpretability in machine learning community. We hope the machine learning methods are safe, interpretable, and they can help us to find meaningful pattern in data. In this paper, we focus on interpretability of deep representation.

We propose a interpretable method of representation based on mutual information, which summarizes the interpretation of representation into three types of information between input data and representation. We further proposed MI-LR module, which can be inserted into the model to estimate the amount of information to explain the model's representation. Finally, we verify the method through the visualization of the prototype network.

1. Introduction

The field of representation learning is developing rapidly (Chen et al., 2020; Grill et al., 2020), but some basic questions such as what is a good representation and what is a general representation are still difficult to answer. Recently, the information bottleneck method has been successfully used to explain neural network's decision (Schulz et al., 2020), which inspired us to use mutual information (Tschannen et al., 2019) to explain and analyze representation learned by neural network. How to interpret and analyze the representation in the neural network, we believe that there should be at least three steps: determining what is encoded in the representation, determining which content in the representation is useful or decision-related, and determining which content is redundant or decision-independent.

2. Related works

Interpreting global representation The popular global interpretable methods are roughly divided into two categories: one is used to visualize convolutional networks, and the other is used to learn the mapping of network decisions/outputs to inputs. Although the second method does not directly explain the representation, we feels that the second category is more similar to the goal of this paper, and werequire a more precise interpretation effect than the first category. We briefly describes the second method: Gradient Maps (Baehrens et al., 2010) and Saliency Maps (Simonyan et al., 2013) are used to calculate the gradient from output neurons to input features. These two methods are very simple and natural, but they cannot be used to explain the decision, they can only explain what is in the neural network, and the value of the gradient is unstable, there will be a lot of noise, Integrated Gradient (**?**) averaging the gradients of multiple inputs, the problem of unstable and noisy gradients of the former is solved. There are many related works such as LRP (Bach et al., 2015a), DTD (Montavon et al., 2017), (Selvaraju et al., 2017) passed output the derivative of the middle feature layer to calculate the weight, and use the weight to assume the activation value to explain it. They also combined GuidedBP to propose GuidedGrad-CAM, which will bring more stable interpretation results.

Interpreting each element of representation Disentangled representation learning want to interpret each factor of representation. They assume that the data changes from independent factors, such as the direction of the image, the intensity of light, and the length of human hair. While changing several factors, other factors may not be affected. They assume that the disentangled representation can easily handle downstream tasks, e.g., when solving gender classification, the learner can make judgments based on the "gender" dimension of the representation. A commonly used method of learning disentangled representations is applied in the implicit representation of vae $z \sim q(z|x)$ constraints, constraints are generally added to the posterior approximation q, the most common objective function can be expressed: $L_{VAE} + \lambda_1(R_1(q(z|x))) + \lambda_2(R_2(q(z)))$, where R_1, R_2 are regularization items, $\lambda_1, \lambda_2 > 0$ is the weight, Higgins et al. (2016) proposes to increase the weight of the kl divergence term $D_{kl}((z|x)||p(z))$ in vae, so that vae can learn the representation with the prior distribution: the specified independent distribution of each dimension, this paradigm has led to many subsequent methods that want to explain the element-level representation. Kim & Mnih (2018) adds a measure to offset the impact after the objective function of vae. For the full correlation term of the variable dependency,

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the objective function is $L_{VAE} + \lambda_2(TC(q(z)))$. The second term is full correlation, which requires density ratio techniques to estimate.

3. Method

3.1. Mutual information estimation

The representation in the neural network encodes the input information. To determine the content contained in the representation, this article can use mutual information theory to calculate the mutual information between the representation $f(x)$ and the input x $I(x, f(x))$, it will tell us how much information about the input is encoded in the represention, but simply knowing $I(x, f(x))$ is not enough, and it's interpretability is poor. For interpretable problems, we generally hope to find a mapping between the interpreted object and the input. For this purpose, we needs to calculate mutual information between the local content x_i of the input x (such as each pixel of the image, each word in the sentence) and the representation $f(x)$, that is to say, we need to know which part of the information in the input data is specifically encoded in the representation. We formalize the amount of information as:

$$\begin{aligned} I(x_i, f(x)) &= E_{x_i}(KL(p(f(x)|x_i)||p(f(x)))) \\ &= E_{x_i}(KL(p(x_i|f(x))||p(x_i))) \end{aligned} \tag{1}$$

We cannot directly calculate the marginal distribution $p(x_i)$, $p(f(x))$ and the conditional probability $p(x_i|f(x)$, conditional probability $p(f(x)|x_i)$ in the formula **??**, these distributions cannot be calculated directly, we use popular information estimation method InforNCE(Tschannen et al., 2019) to estimate $I(x_i, f(x))$, let $z = f(x)$, then the mutual information between local input and representation is:

$$I(x_i, f(x)) \geq E(\frac{1}{N \cdot K}\sum_{j=1}^{K}\sum_{i=1}^{N} log\frac{e^{f(x_i^j, z^j)}}{\frac{1}{N \cdot K}V}) \tag{2}$$

$$V = \sum_{m=1}^{K}\sum_{n=1}^{N} e^{f(x_m^n, z^j)} \tag{3}$$

Where N is the number of local inputs for each sample (the number of pixels in the image, the number of words in the sentence), and j represents the total number of samples/the total number of samples in the batch. Although there are many mutual information estimation methods (Hjelm et al., 2018; Belghazi et al., 2018), InforNCE is a low variance estimation method, which is widely used in representation learning.

3.2. Information bottleneck

We now need to extract useful information or decision-related information in the representation. As long as the representation contains this information, the decision of the model will not be affected. To extract useful information or decision-related information, naturally, this article needs Use the information bottleneck principle (Tishby & Zaslavsky, 2015), let y represent the label, the information bottleneck principle is a learning principle to obtain the minimum amount of information, and the general formal description is to maximize the mutual characterization of z and label y At the same time of information, it reduces the mutual information between the characterization z and the input x. Its usual optimization goals are:

$$\max I(z, y) \quad s.t.\ I(x, z) \leq c \tag{4}$$

After introducing the Lagrange multiplier β, we have

$$\max I(z, y) - \beta I(x, z) \tag{5}$$

We follow the approach of (Schulz et al., 2020), only optimize the second item of the formula (6), and replace the first item of the formula (6) with the objective function of the original model. This is intuitive approximation, in the learning process of the neural network, the label information is continuously encoded in the representation. In order to extract the useful part of the representation in a certain model, we need to optimize:

$$L(x) = \max l(x) - \beta I(x, z) \tag{6}$$

Where l(x) is the original objective function of the model. Similar to the previous section, this article cannot directly optimize the formula (6). Its interpretability is not good. We need to specifically extract useful information from the local input. We optimize:

$$L(x) = \max l(x) - \beta \sum_{i=1}^{N} I(x_i, z) \tag{7}$$

We need to use the method of estimating the upper bound of mutual information to optimize the formula 7. At present, there is no reliable method of estimating the upper bound of mutual information. This article can only select the experimentally reliable method The VIB method (Alemi et al., 2016) is used to optimize the formula (7). In this paper, the variational distribution q is used to replace the marginal distribution p in the formula **??**, then we have:

$$I(x_i, z) \leq E_{x_i}(KL(p(z|x_i)||q(z))) \tag{8}$$

3.3. Information redundancy

We now need to identify the redundant information in the representation. The redundant information is a kind of information that is irrelevant to the decision. Removing it will not affect the decision of the model. We first calculate the mutual information between the input and the representation $I(x, z)$, and then calculate the useful information/decision-related information $I(x, z^{'})$ in the representation. Finally, we use the difference between the two to represent the amount of redundant information in the representation. As before, we specifically calculate the amount of redundant information in the local input:

$$R = \sum_{i}^{N} I(x_i, z) - I(x_i, z^{'}) \tag{9}$$

In order to find three kinds of information in a specific model to analyze representation, we need to combine them with the original objective function of the model and then learn to get it. We add the formula (3) and the formula (8) in the original objective function, the total objective function is:

$$\begin{aligned} &L(x) = \max l(x) \\ &+\alpha E_{x_i}\left(\frac{1}{K}\sum_{j=1}^{K} log \frac{e^{f(x_i^j, z^j)}}{\frac{1}{N \cdot K}\sum_{m=1}^{K}\sum_{n=1}^{N} e^{f(x_m^n, z^j)}}\right) \\ &-\beta E_{x_i}(KL(p(z|x_i)||q(z))) \end{aligned} \tag{10}$$

where α and β are hyperparameters. In a specific model, according to (10), we can get the three kinds of information we want to explain the representation after optimizing.

3.4. MI-LR module

In order to estimate the above three kinds of information in the model, we design the MI-LR module to insert into the model to calculate the objective function (10) conveniently, and then estimate the amount of information. Figure 1 shows the overall architecture of the MI-LR module. The MI-LR module includes three small modules to achieve the functions we want. We realize what we want by adding these three small modules to the original model. The function of estimating the amount of information, and then we will separately introduce how each function is implemented, and how to calculate the objective function and the three kinds of information.

In fact, we cannot calculate the amount of information between the local input and the representation, because the local input always has low dimension, e.g., each pixel of the image is represented by one or three dimension. We need to calculate the amount of information between local features and representation in the model instead of calculating the amount of information between local input and representation.

3.4.1. Information estimate

We use the Informax-estimator module in the figure 1 to estimate the mutual information in the formula (3), which can be implemented simply by a single-layer or two-layer mlp, which will participate in the calculation of the local features converting to the same dimension as the global representation, and then calculate the lower bound of the mutual information between the two according to the formula (3). As shown in 1, after inserting the MI-LR module, the local feature x_{ij} and the representation z will be sent to the Informax-estimator module, and then follow the formula 3 to obtain the mutual information between local features and representation, and use it as a part of the objective function (10).

3.4.2. Information bottleneck

We use the Infor-bottleneck module and mask module in the figure 1 to realize the information bottleneck.

The Infor-bottleneck module can be simply implemented by a single-layer or two-layer mlp, which converts the local features and representation involved in the calculation to the same dimension, and then calculates the upper bound of the mutual information between the two according to the formula 8. The mask module is used to assist in the realization of the information bottleneck function. Like (Schulz et al., 2020), it consists of several convolution layer whose kernel size is 1. After inputting local features, the mask α can be automatically inferred, whose dimension will be the same as the input local features, the mask α will occludes local features.

How to reduce the mutual information between local features and representation and realize the information bottleneck function? We refer to and modify the implementation in (Schulz et al., 2020). In the first stage, we first make the input X_i get the global representation z_i through the original model, and then collect the features of each layer in the network . In the first stage, we first let the input X_i get the global representation z_i through the original model, and then collect the features of each layer in the network. In the second stage, we insert the Infor-bottleneck module and the mask module into the original model, pass X_i through the original model again to obtain local features x_i, and then use the features collected in the previous stage, we send it to the mask module to get the mask α, $\alpha \in [0, 1]$, the dimension of α_j is the same as the local feature x_{ij}, and then x_i is multiplied by α to get the occluded local feature $x_i^{'}$, and finally $x_i^{'}$ and z_i are sent to the calculation formula 8 in the Infor-bottleneck module to obtain useful information/decision-related information in the representation, and also participate in the optimization as a part of the objective function 10

It can be imagined: α is automatically learned by the mask module. When α is all 1, the original value is retained between $x_i^{'}$ and z_i The amount of information, namely: $I(x_i, z_i) = I(x_i^{'}, z_i)$, when α is all 0, $x^T here is no more mutual information between'_i$ and z_i.

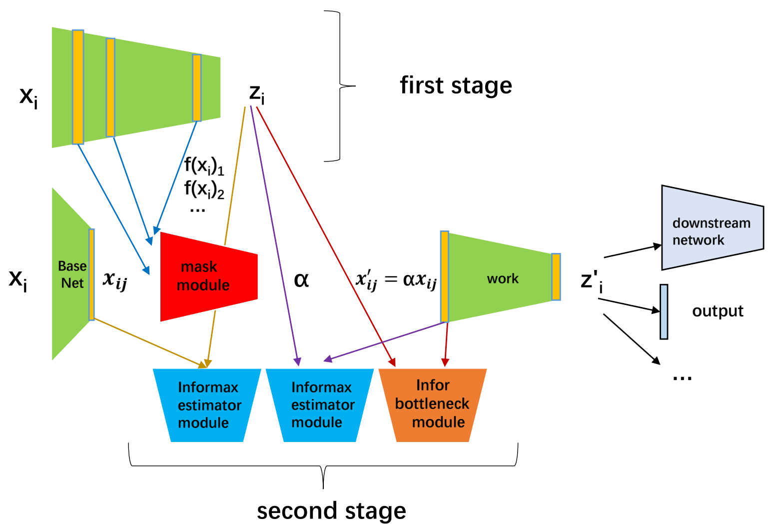

Figure 1. MI-LR module

Under normal circumstances, part of the value of α will be approximately equal to 0, which reduces the mutual information between local features and representation. It means we realize the information bottleneck principle and extract useful information/decision-related information in the representation.

3.4.3. Information redundancy

In the previous step, we got the original local feature x_i, the occluded local feature $x_i^{'}$ and the representation $z_i^{'}$, we send them to the Informax-estimator module, and use the formula 9 to calculate the amount of redundant information. The amount of redundant information does not need to be added to the objective function to participate in optimization.

4. Experiment

Different from other interpretability methods (Baehrens et al., 2010; Bach et al., 2015b; Schulz et al., 2020), we focus on analyzing and explaining the representation of the model. We can use three kinds of information to get profound interpretation results. We use a typical prototype network as an example to illustrate how to explain and analyze the representation of the model using the methods we proposed.

4.1. Prototype Network Visualization

The prototype network is a typical few-shot learning method. The typical learning task of few-shot learning is as follows: Given a query image and a support set composed of multiple types of images, few-shot learning method is to assign the query image to the support which is concentrated in the appropriate category. According to the number of samples in each category and the number of categories in the query image and support set, few-shot learning will be divided differently, such as: 5way1shot, 5way5shot. The prototype network uses the prototype concept for assignment. For a good visualization effect, we will set the learning way is 5way1shot, that is: there will be 5 types of samples in the support set, and each type of sample will have 1 image, and we also specify 5 query samples: Selecting 1 picture as the query sample from each category in the support set. The figure 2 is an example. The support/query above each column represents whether the 5 samples in the column belong to the query sample or the support set.

We first train the prototype network, after training the prototype network, we fix its parameters to prevent subsequent changes, and then insert the MI-LR module into the layer1 block and avgpool layer of the residual network as the feature extractor, layer1 block's output of is used as a local feature, and the output of avgpool is used as a representation. The MI-LR module will learn the parameters and calculate the amount of information in the way shown in the figure 1. Finally, we will get three kinds of information betweenn the output of the layer1 block and the avgpool layer. We visualize these three kinds of information and explain representation: the output of avgpool layer. The three types of information can tell us what content is encoded in the representation of the query sample and the support set sample when the prototype network is learning, so that we can know how the prototype network is distinguished. We will visualize the original image first, and then visualize the heat map of the three output information and the mixed image of the original image and the heat map.

4.1.1. Dataset

For a good visualization effect, we use the bird dataset CUB-200-2011(Wah et al., 2011). It is more suitable for visualization than general image data sets.

4.1.2. Mutual Information Visualization

The picture 2 is the original image, the picture 3 is the heat map of mutual information, and the picture 4 is the mixed picture of the heat map and the original picture. According to the previous sections: the mutual information between the representation and the local input represents how much input information the representation contains. The red part of the heat map is the part with high information. From the heat map 3, when the prototype network is performing a few-shot learning task, the avgpool layer of the prototype network almost contains all the input 2 except for the background also contains noise such as branches. Different parts have different amounts of information, and the amount of information on the chest of a bird is low.

This is similar to general intuition. The avgpool layer has a higher dimension and a large capacity enough to encode most of the image in the CUB dataset. Combined with the original image, we can see a better interpretation effect from the mixed image 4.

4.1.3. Visualization of decision-related information

Figure 5 is a mixed image of the original image and the heat map of decision-related information. According to the previous sections: the decision-related information between the representation and the input represents the input information contained in the representation that makes the decision sufficient. The activation area of figure5 is very small, which shows which part of the input coded in the representation is the most important for decision-making. We can see: the bird's mouth, the unique feathers on the body When the prototype network performs the discrimination task, these areas are the main basis for the prototype network. Unlike the InforNCE estimation method, the VIB method estimates a large degree of dispersion of information, and it is very suitable for estimating decision-related information, because we need as few activation regions as possible to determine the most important input information contained in the representation, but unfortunately the VIB method is very inaccurate. Although its visualization effect is very good, the VIB method needs to specify the confirmed variational distribution, which affects it's estimation accuracy.

4.1.4. Visualization of Redundant Information

The picture 6 is a mixed picture of the heat map of the redundant information between the output of the layer1 block and the output of the avgpool layer and the original image. According to the previous sections: the redundant information in the representation refers to the input information encoding in the representation which is redundant for decision-making, removing it does not affect the decision-making. Our visualization effect is not ideal, but we can still find that the active area of redundant information is mainly the tail and back area of the bird. These areas have no effect on distinguishing the type of bird.

5. Conclusion

We propose a representation interpretation method based on mutual information, which summarizes the interpretability of the representation into three types of information between the local input data and the representation, and further proposes the MI-LR module, which can be inserted into the model to calculate the amount of information to explain the representation of the model. Finally, the interpretation ability is visually demonstrated through the visualization of the prototype network.

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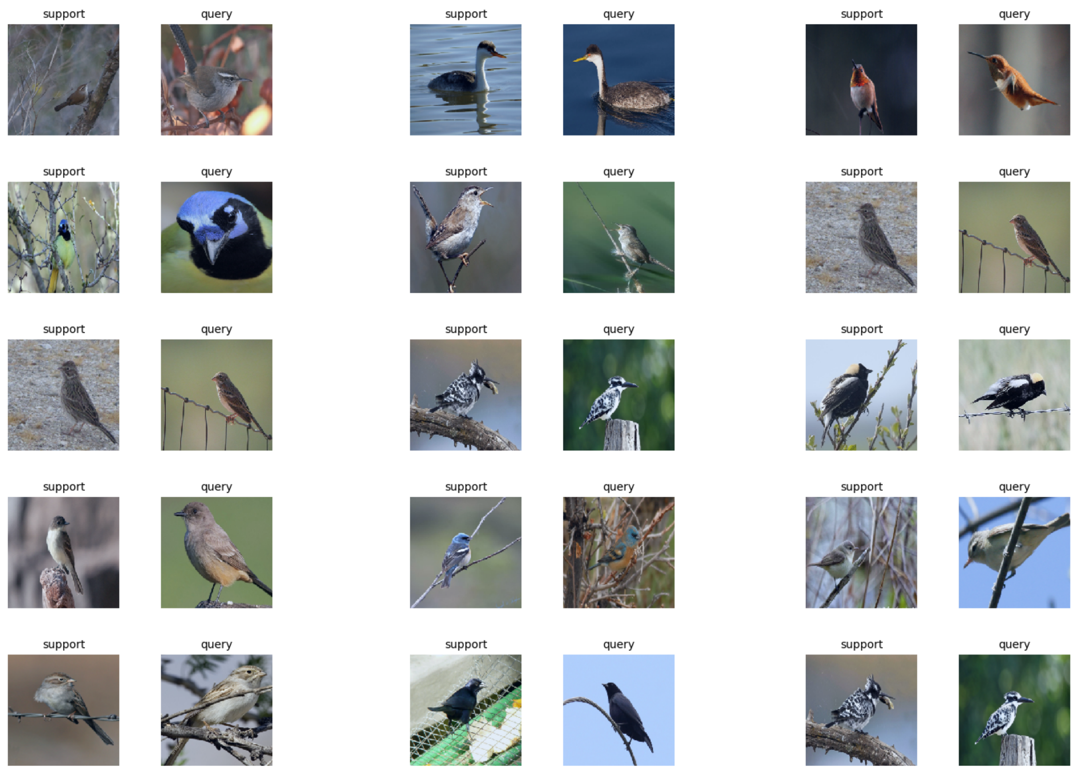
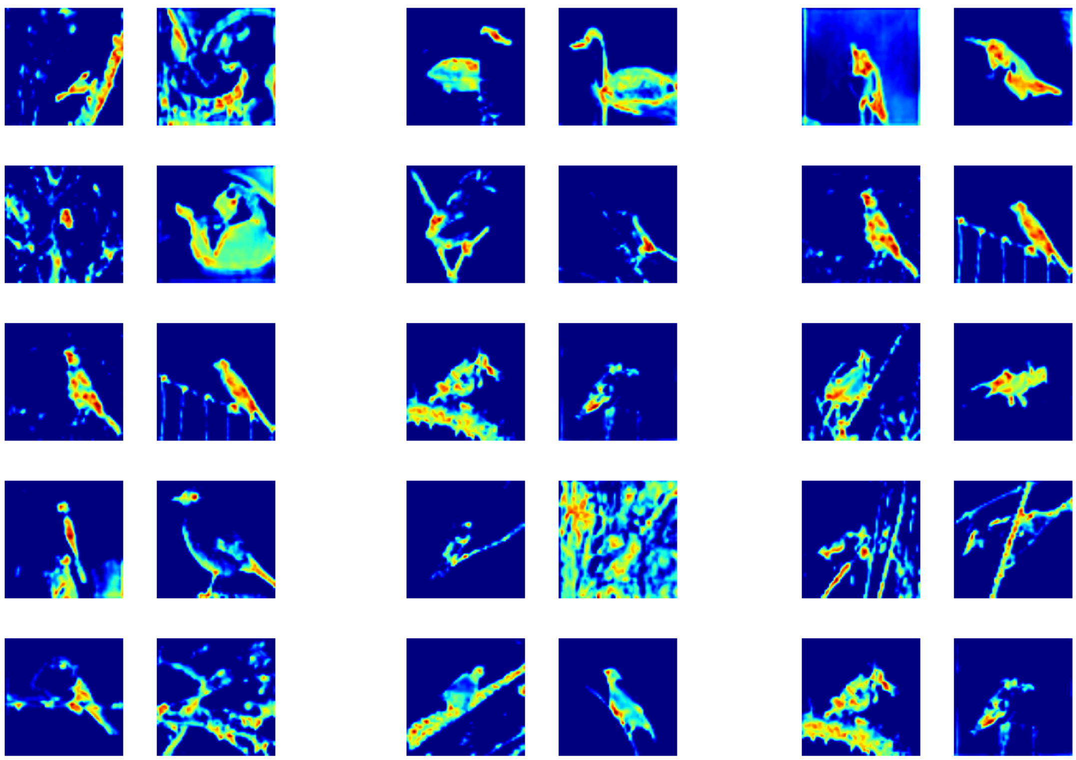


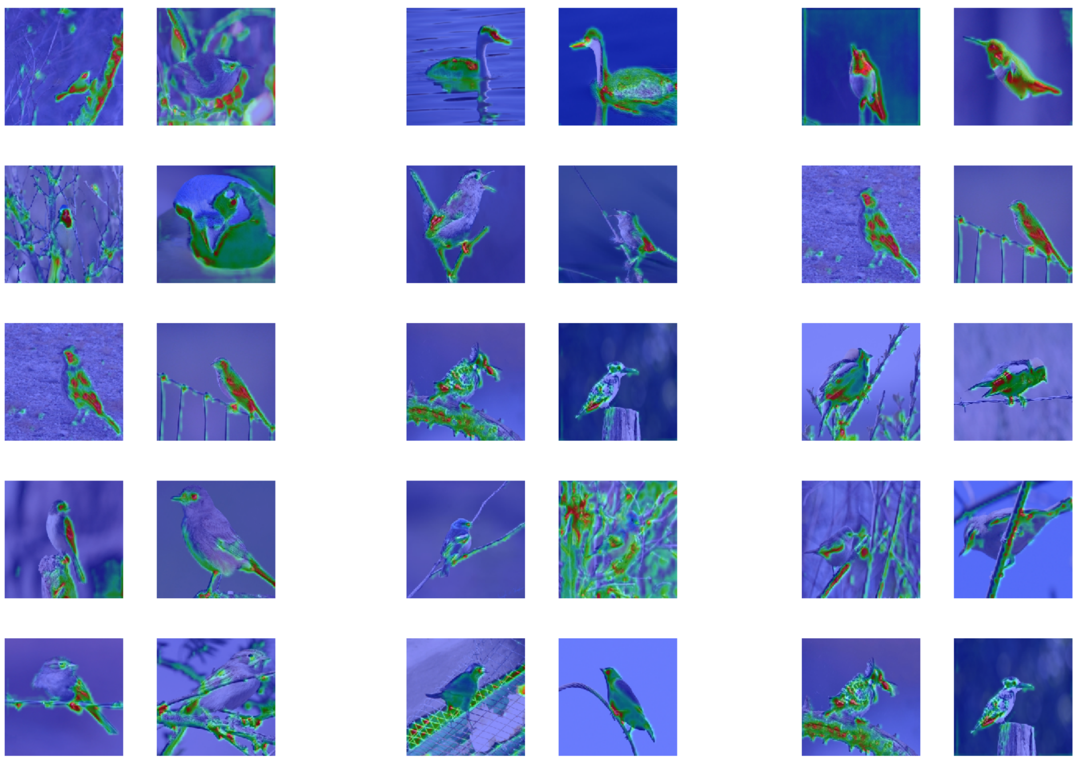
(a) (b) (c)

Figure 2. original image



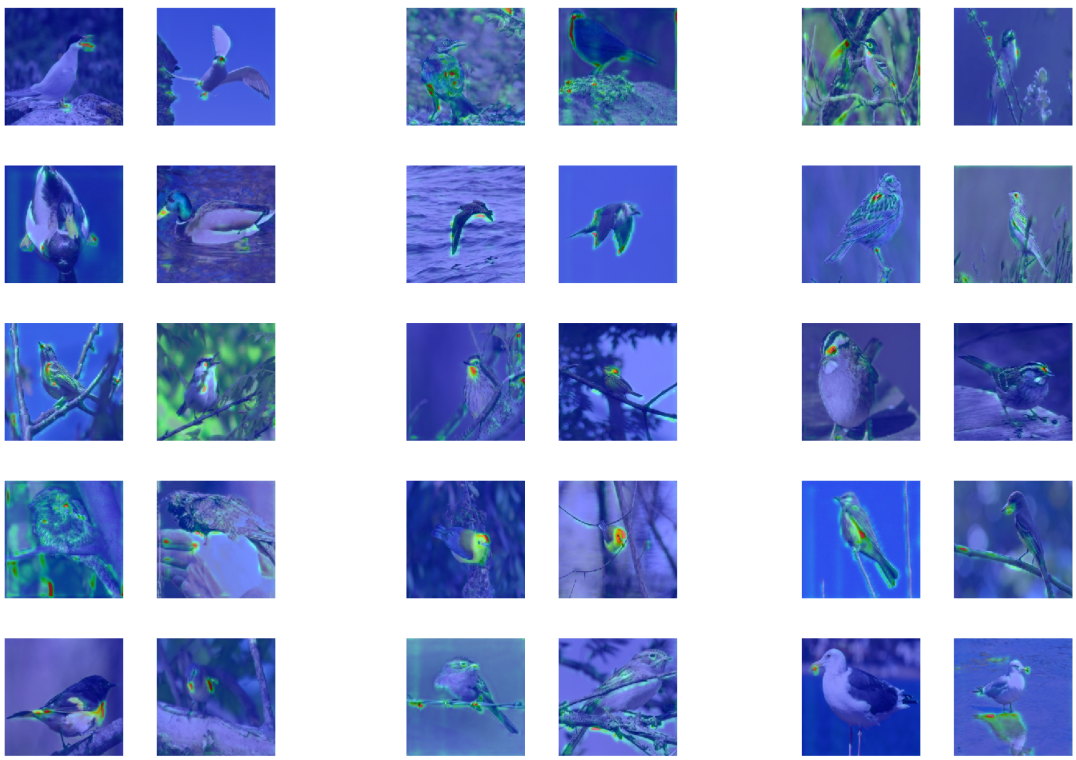
(a) (b) (c)

Figure 3. heat map of mutual information



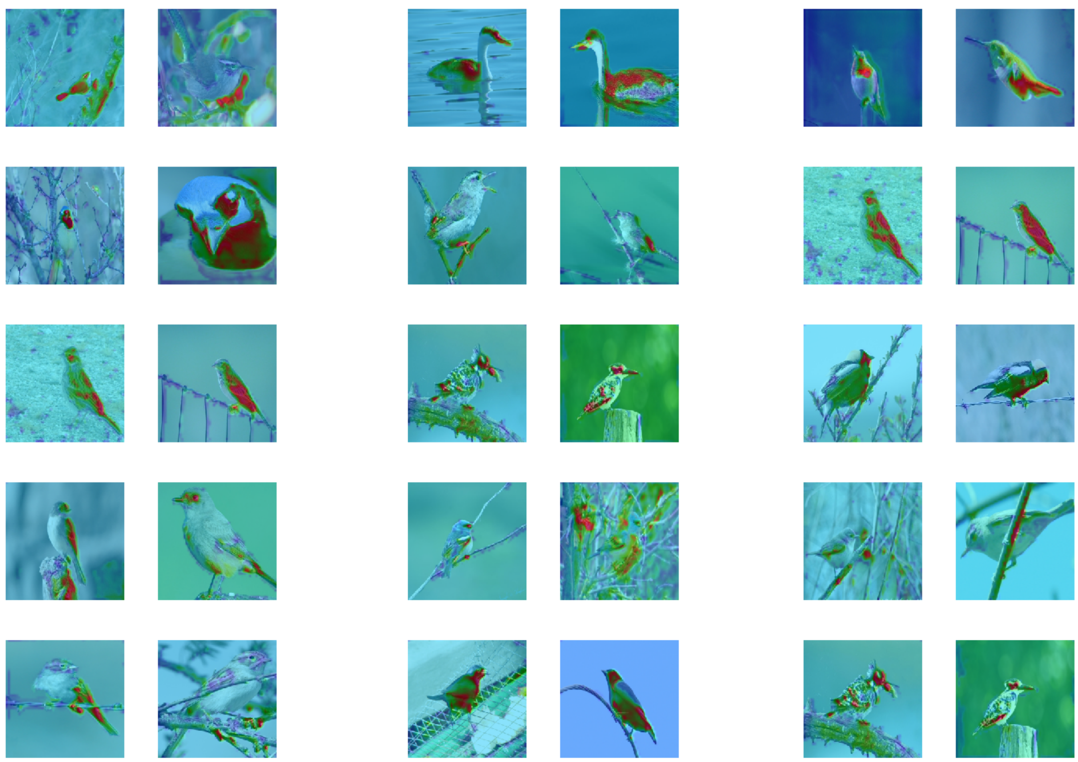
(a) (b) (c)

Figure 4. mixed figure between heat map and original figure of mutual information



(a) (b) (c)

Figure 5. mixed figure between heat map and original figure of decision-related information



(a) (b) (c)

Figure 6. mided image between heat map and original image of redundant information

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