
An Information-theoretic Progressive Framework for Interpretation

Zhengqi He

Lab for Neural Computation and Adaptation, RIKEN Center for Brain Science, Japan
 zhengqi.he@riken.jp

Taro Toyoizumi

Lab for Neural Computation and Adaptation, RIKEN Center for Brain Science, Japan
 Department of Mathematical Informatics, Graduate School of Information Science
 and Technology, The University of Tokyo
 taro.toyoizumi@riken.jp

Abstract

Both brain science and the deep learning communities have the problem of interpreting neural activity. For deep learning, even though we can access all neurons' activity data, interpretation of how the deep network solves the task is still challenging. Although a large amount of effort has been devoted to interpreting a deep network, there is still no consensus of what interpretation is. This paper tries to push the discussion in this direction and proposes an information-theoretic progressive framework to synthesize interpretation. Firstly, we discuss intuitions of interpretation: interpretation is meta-information; interpretation should be at the right level; inducing independence is helpful to interpretation; interpretation is naturally progressive; interpretation doesn't have to involve a human. Then, we build the framework with an information map splitting idea and implement it with the variational information bottleneck technique. After that, we test the framework with the CLEVR dataset. The framework is shown to be able to split information maps and synthesize interpretation in the form of meta-information.

1 Introduction

Development in computational power, big data techniques, and better algorithms within the last decade has seen a great leap in brain-inspired artificial-intelligence techniques, namely Deep Neural Networks (DNN) [13]. DNN has made great achievements in fields such as image recognition [26], speech recognition [17], natural language processing [41], game playing beyond human-level performance [36]. On the other hand, being one of the most famous black-box models, its failure under certain circumstances, with the adversarial attack being one of the most famous examples [14], starts an increasing trend of interest in research into the black-box model interpretation. Further, interpretation for models like DNNs is also favorable, for example, for explaining model behavior, knowledge-mining, ethics, and trust. [10, 30]

Even though plenty of discussions have emerged about model interpretation in recent years, people have different ideas about the definition and methods for interpretation under different circumstances. Concerning when to interpret, there are post-hoc style and transparent style [30]. Post-hoc style interpretation tries to separate the model training step and model interpretation step. This style is favorable since people can focus on maximizing a model's performance and worry about interpretation later. However, since model training and interpretation phases are decoupled, the interpretation fidelity is not guaranteed [12]. Transparent style methods are designed to be interpretable but are often

relatively less competitive in prediction performance. Concerning the applicability of interpretation methods, there are a model-specific type, targeting a certain class of models, and a model-agnostic type, where the interpretation method doesn't depend on the model [3]. Concerning explanation scope, there are global explanation v.s. local explanation, where global explanation gives information about how the task is solved in general while the local explanation is more focused on certain examples or certain parts of the model [10]. With respect to the form of interpretation, there is even larger variety, just some non-complete examples, such as information feature [7], relevance feature [4], hot spot of attention [19], gradient information [37], easier models like discrete-state models [18], shallower decision trees [11, 44], graph models [47], or less number of neurons [27]. The readers can refer to [3] for more complete overviews.

With such a diversity of works around the idea of interpretation, we still believe that the current discussion lacks generality and doesn't touch the core idea behind the interpretation. By rethinking the fundamental property of interpretation and starting from intuitive assumptions, we build a general framework to synthesize interpretation from an information-theoretical perspective. The proposed framework is transparent in style, capable of both global and local explanation, and produces interpretation in the form of meta-information. The framework is then implemented to solve image recognition tasks on a simplified CLEVR dataset in an interpretable manner [23].

2 Towards a Theoretical Framework for Model Interpretation

Lacking a solid theoretical framework for interpretation would hinder the development of a better intelligent system. Take DNN as an example; all mysterious behavior and troubles of DNN somehow related to lack of interpretation of their internal working mechanism. Thus, having a well-defined theoretical framework for model interpretation is strongly desired. This section discusses intuitions from everyday experience seeking the foundation to build the theoretical framework for interpretation.

2.1 Interpretation as Meta-Information

It is safe to assume that all neural network models are information processing machines. Assume X to be input random variables, Z to be output random variables. The interpretation of model decision can then be viewed as a problem to explain its information processing. For example, if Z is a yes-or-no decision with equal probability, then 1 bit of information is sufficient from input X to extract the answer. A full interpretation requires an end-to-end tracking of this 1 bit of information. Since we're handling computational models, we can also assume all intermediate information is available to us. As a result, for any intermediate random variable Y , the flow of mutual information $I(X; Y)$ and $I(Y; Z)$ are calculable in principle. Then, the interpretation would come out from this pattern of information flow.

However, being able to track this information flow is not yet enough. One obvious problem is that information by itself is meaningless since meaning is also a kind of information that describes the information. This kind of information is usually named meta-information. Considering a coin-tossing example, if someone is tossing a coin, 1-bit per toss amount of information is generated. However, this generated information is meaningless to you unless you know that this information will be used, for example, to draw a lottery. In fact, needs for meta-information are ubiquitous, ranging from a digit inside a spreadsheet to computer file-system, internet protocol, WiFi standard, and so on. In neuroscience, recording neural activity alone is not enough to understand the brain. It is not until we assign proper meta-information to the information conveyed by the neurons (for example, we know the activity of place cells in the hippocampus is related to positions [31]) that we can understand what the neurons are doing.

Let's go back to the model. Meta-information of the intermediate information flow is not needed to solve the problem but is crucial for interpreting what the model is doing. As a result, this meta-information doesn't necessarily come from the task dataset (i.e., the pairs of inputs and outputs). We noticed that a good source for this meta-information is the task itself, and we will describe how in the following sections.

2.2 Progressive Nature of Interpretation

In this section, the authors want to emphasize an important property of interpretation: interpretation is progressive. In other words, background knowledge should be provided in advance to deliver understandable interpretation [8, 5]. Learning in a progressive context is not a rare setting in machine learning [2, 34, 32], and usually named "lifelong learning", "sequential learning" or "incremental learning". In one example [24], the authors point out that interpretability emerges when lower-level modules are progressively made use of. However, it is relatively underrepresented in current literature about the role of progressiveness in model interpretation.

Interpretation usually involves a human audience, whose background crucially affects whether it makes sense. Consequently, to judge interpretation quality, a large human-annotated dataset [24] is usually needed. This complicates the problem as there is often no objective definition of the target audience. A natural question is whether it is possible to move humans out of the loop when synthesizing an interpretation. The idea of defining an audience-model is discussed in [9], in which interpretability depends on the model instead of a human audience.

Combining these two ideas, we design the interpretation synthesis framework as a progressive framework over a sequence of tasks where the interpretation of later tasks is synthesized based on a model that has been trained on earlier tasks.

2.3 Interpretation Design Patterns

In this section, we'll talk about other useful design patterns of the framework for interpretation.

Interpretation in right level: Consider a complex model, especially industry-level DNNs whose number of hidden variables can easily surpass hundreds of millions, parameter-by-parameter fine-grain information interpretation is neither possible nor necessary. One feasible solution to this problem is decreasing the interpretation resolution and find the right level for interpretation. One of the most famous examples of "interpretation at the right level" is statistical mechanics. To understand the behavior of gas, we don't need to track every particle. What we really care about are higher-level properties such as temperature and pressure. We choose interpretation in the level of tasks in our framework.

Inducing independence: Interactions between random variables cause redundancy/synergy of information [42], which will elevate complexity for information flow analysis. Inducing independence among variables via model inductive bias can be helpful to ease this problem. Useful methods are widely available in ML fields such as independent component analysis [20] and variational auto-encoders [25].

Markovian: Considering the situation where some intermediate random variable Y forms a complete cross-section of the information flow, so that $X \rightarrow Y \rightarrow Z$ forms a Markov chain. If it is the case, $X \rightarrow Z$ can be explained serially by $X \rightarrow Y$ and $Y \rightarrow Z$. The data-processing inequality of mutual information holds in this case: if $X \rightarrow Y \rightarrow Z$, then $I(X; Y) \geq I(X; Z)$ and $I(Y; Z) \geq I(X; Z)$, which means any piece of information about X not included in Y would not be available anymore for the downstream. With the help of Markovian property, we can reduce the problem of interpretation to the problem of tracking the amount of mutual information flow through a certain number of cross-sections without worrying about the specific form of the transformation that happens in-between each cross-section.

To conclude, the interpretation we are going to synthesize by our framework would be the meta-information describing the amount of information needed from each previously experienced task to solve the current task. We will formalize the idea in the language of information theory in the following sections.

3 The Progressive Interpretation Framework

In this section, we start building the abstract framework for interpretation following the discussions above. Assume we have a model with stochastic input X , which is assumed statistically the same regardless of a task, and stochastic output label Z . The internal representation of the model is Y . Thus, they form a Markov chain $X \rightarrow Y \rightarrow Z$. The model starts with Task 1 and finds out that it minimally needs $I(X; Y_1)$ amount of information and the corresponding representation Y_1

to solve Task 1. Then, the model augments the minimal representation Y_{else} ideally independent of Y_1 , i.e., $I(Y_1; Y_{\text{else}}) = 0$, to auto-encode the input X . Thus, the joint internal representation is $Y = \{Y_1, Y_{\text{else}}\}$. The interpretation comes in when the model tries to perform Task 2 using the representation learned previously. The model finds out a minimum representation $Y_{(1;2)}$ from Y_1 that is useful to solve Task 2. Unless Task 2 is a sub-task of Task 1, the information in Y_1 alone is insufficient to perform Task 2. The rest of the information can be found in Y_{else} since Y_1 and Y_{else} jointly represent the input. The model also finds the minimal representation $Y_{(\text{else};2)}$ from Y_{else} that is useful to solve Task 2. Then we ideally have $I(X; Z_2) = I(Y_{(1;2)}, Y_{(\text{else};2)}; Z_2)$, where Z_2 is the output for Task 2. The meta-information of how much information is needed from Y_1 and how much information is needed from Y_{else} is defined as the progressive interpretation in our framework. After Task 2, the model could further update its input representation into $Y = \{Y_1, Y_2, Y_{\text{else}'}\}$, where $Y_2 = Y_{(\text{else};2)}$ and the remaining part is updated to $Y_{\text{else}'}$, excluding Y_2 from Y_{else} . The model is then ready for the next iteration.

In general, the progressive interpretation framework is formalized as follows:

1, Assume after Task n , a model has a minimal internal representation $Y = \{Y_1, Y_2, \dots, Y_n, Y_{\text{else}}\}$ that encodes the input X . The optimization in the ideal case yields independence among the previous task-relevant partitions:

$$I(Y_i; Y_j) = 0, (i \neq j \in [1, n] \cup \text{else}).$$

2, Then, the model is faced with new Task $n + 1$, and learns to output Z_{n+1} . After learning Z_{n+1} , the model distils the necessary part $Y_{(i;n+1)}$ from each partition $Y_i (i = [1, n] \cup \text{else})$ for solving Task $n + 1$. This is achieved by minimizing

$$I(Y_{(i;n+1)}; Y_i), (i \in [1, n] \cup \text{else})$$

while maintaining the best task performance, i.e., by maintaining ideally all the task relevant information:

$$I(\bigcup_{i=1}^{n,\text{else}} Y_i; Z_{n+1}) = I(\bigcup_{i=1}^{n,\text{else}} Y_{(i;n+1)}; Z_{n+1}).$$

3, The interpretation is defined as the meta-information of how much the individual partitions $\{Y_i\}$ for previous tasks $i = [1, n] \cup \text{else}$ are utilized to solve Task $n + 1$. Namely, the composition of the mutual information $I(Y_{(i;n+1)}; Y_i)$ over the different partitions $i = [1, n] \cup \text{else}$ is the meta-information we use to interpret the global operation of the neural network. Then, local interpretation for each example is available from $\{Y_{(i;n+1)}\}$.

4, After Task $n + 1$, the model updates the representation map by splitting Y_{else} into the newly added representation $Y_{(\text{else};n+1)}$ and its complement $Y_{\text{else}} \setminus Y_{(\text{else};n+1)}$. Then, the former is denoted as Y_{n+1} and the latter is denoted as $Y_{\text{else}'}$. The model would continue this for further iteration and interpretation of the tasks. The process can be illustrated in Fig. 1

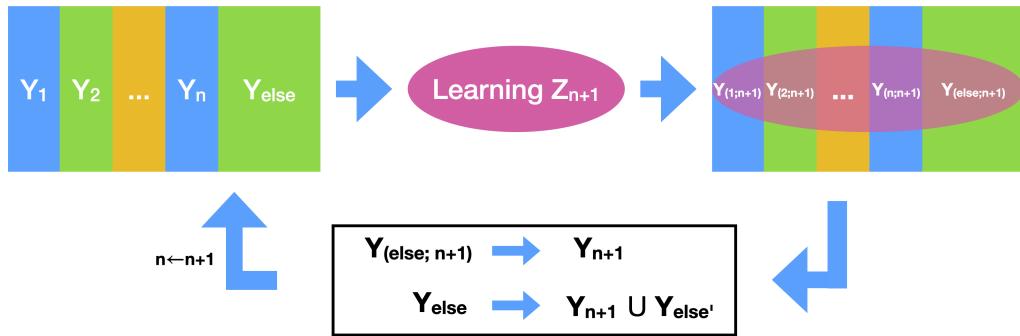


Figure 1: Information diagram for the progressive interpretation framework.

4 Neural Network Implementation of Progressive Interpretation

Neural network implementation of progressive interpretation can mainly be divided into two steps. In step 1, a network is trained on Task 1. After that, we need to split the representation map into Task

1 related part and unrelated part with information bottleneck (IB) [38]. In step 2, Task 2 comes in, and interpretation is gained by knowing how much information is needed from each sub-region. By adding new tasks and looping over step 1 and step 2, progressively more informative interpretation can be gained. The information flowing graph we are going to implement in the following sections is shown in Fig. 2.

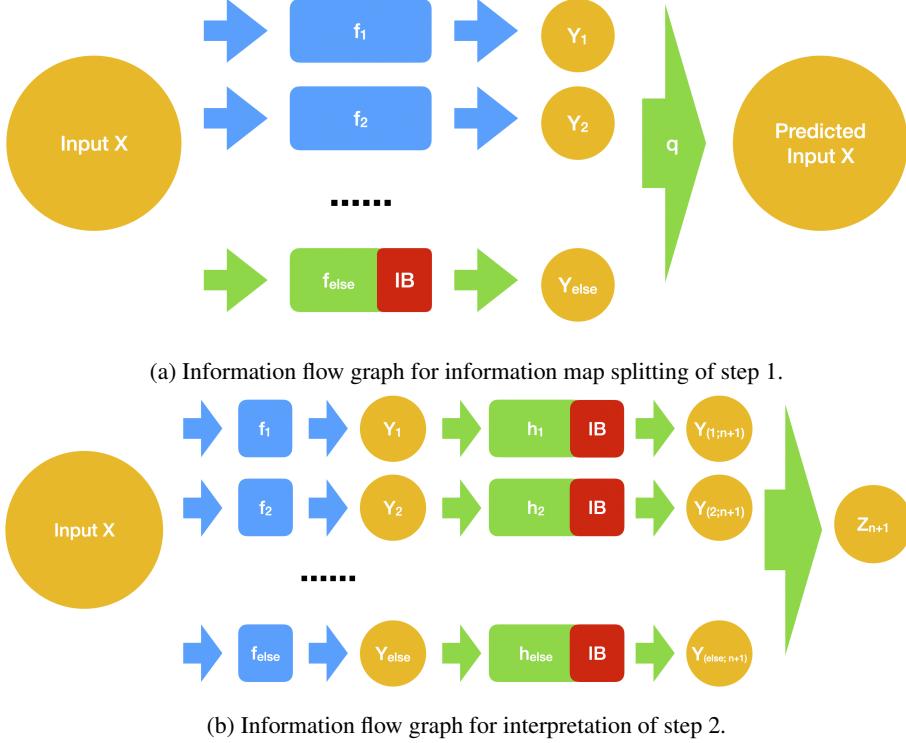


Figure 2: Information flow graph of the progressive interpretation framework. Yellow circles are representations, green/blue arrow (and square) represents neural networks. Green ones are put under training while blue ones are fixed. Red square with IB represents information bottleneck.

4.1 Step 1: Task 1 Training and Information Map Splitting

Our particular interest is in the neural network style model interpretation, for its black-box nature and close relationship to the human brain. Since our framework is information-theoretic, it does not depend on any specific type of neural network. All neural networks, independent of their types, are treated as segments of the information processing pipeline, which maps input random variables to output ones. Which type of neural network to choose is decided by the specific problem.

Suppose a new model with task input X is faced with its first task and learns the network output to approximate label \tilde{Z}_1 . It is not difficult to train a neural network for this task by optimization:

$$\min_{\theta} D(f_{1,\theta}(X) || \tilde{Z}_1)$$

D is a distance function, such as KL-divergence or mean-square error, which is decided by the problem itself. After training, we will be able to obtain the representation of Task 1 as $Y_1 = \text{Sample}[f_1(X)]$, where f_1 indicates $f_{1,\theta}$ with the optimized parameters θ . The function $\text{Sample}[f_1(X)]$ represents sampling the calculated probabilistic distribution parameterized by a neural network output f_1 for each realization of the input X . The form of the probability distribution depends on the modality of the label \tilde{Z}_1 as we introduce below with an example. Note that the coarse-graining of Y_1 by the sampling is important for making Y_1 to be specifically relevant to Task 1. Because without the sampling, $f_1(X)$ as a non-linear mapping of X inevitably contains some Task 1 unrelated features of X , which could be used to solve other tasks. These Task 1 unrelated features are typically small and

can be masked by the coarse-graining due to the sampling. In a neural network, sampling is usually implemented with the reparameterization trick [25] described later.

Then, our next problem is how to obtain Task 1 unrelated representation Y_{else} , which ideally satisfies $I(Y_1; Y_{\text{else}}) = 0$, to complement the intermediate representation about the input. Here, we argue that Y_{else} can be obtained via the implementation of IB on an auto-encoding problem:

$$\max_{\theta} [I(Y_1, Y_{\text{else}}; X) - \gamma I(Y_{\text{else}}; X)], Y_{\text{else}} = \text{Sample}[f_{\text{else}, \theta}(X)], \quad (1)$$

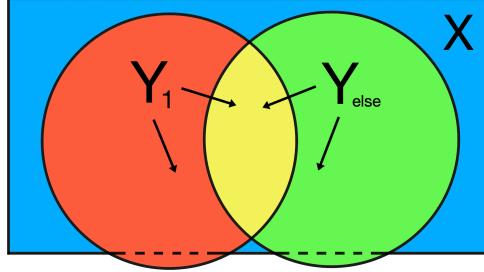


Figure 3: Information diagram for representation map splitting during the training of $f_{\text{else}, \theta}$.

where γ is the scaling factor controlling the trade-off between including and excluding different information, which should be larger than 0 and smaller than 1. Note that the learned f_1 function is fixed while $f_{\text{else}, \theta}$ is trained. Reading from the information diagram in Fig. 3, Y_1 (region red and yellow) is mostly within X (square box) but partly outside of X due to the sampling. The same thing applies to Y_{else} (region green and yellow). The region yellow is within the box because sampling noise for Y_1 and Y_{else} is independent. With Y_1 fixed, Eq. 1 is trying to maximize the region red, yellow, and green within the box while minimizing with less priority the region yellow and green within the box by modifying Y_{else} (boundary surrounding green and yellow). As a result, the mutual information $I(Y_1; Y_{\text{else}})$ (region yellow) will be minimized, and the region green will cover the region light blue.

We choose the variational information bottleneck implementation [1, 29]: Loss function

$$L(p, q, r) = \mathbb{E}_X \left\{ \mathbb{E}_{Y_1|X} \mathbb{E}_{Y_{\text{else}}|X} [-\log q(X | Y_1, Y_{\text{else}})] + \gamma \text{KL}[p(Y_{\text{else}} | X), r(Y_{\text{else}})] \right\} \quad (2)$$

is used to optimize encoding distribution $p(Y_{\text{else}} | X)$, decoding distribution $q(X | Y_1, Y_{\text{else}})$, and the prior distribution $r(Y_{\text{else}})$ for p . During the optimization, \mathbb{E}_X is computed by averaging over N training samples of input $\{x_j | j = 1, \dots, N\}$. $\mathbb{E}_{Y_1|X}$ is computed by sampling the internal representation for Task 1, $Y_1 = \text{Sample}[f_1(X)]$, with the trained and fixed f_1 . $\mathbb{E}_{Y_{\text{else}}|X}$ is computed by sampling $Y_{\text{else}} = \text{Sample}[f_{\text{else}, \theta}(X)]$ from the encoding distribution $p(Y_{\text{else}} | X)$ that depends on $f_{\text{else}, \theta}$. Y_{else} can be a vector of either continuous or discrete variables [29] but, for the ease of mutual information calculation, we assume that Y_{else} is a vector of binary elements and p and r are multi-dimensional Bernoulli distributions. Another merit for multi-dimensional Bernoulli distribution is that we can regularize the prior distribution's entropy to induce sparsity and make the following analysis easier, which is usually not the case for continuous prior such as multi-dimensional Gaussian. Specifically, we use the Gumbel-Softmax reparameterization trick [22] to draw samples from the multi-dimensional Bernoulli distribution without blocking gradient information. The d th element of Y_{else} is given by:

$$[Y_{\text{else}}]_d = \text{Sigmoid} \left[\left(\log \frac{[f_{\text{else}, \theta}(X)]_d}{1 - [f_{\text{else}, \theta}(X)]_d} + \Delta g_d \right) / \tau \right] \quad (3)$$

where $\text{Sigmoid}[x] = 1/(1 + e^{-x})$ is the Sigmoid function, τ is a temperature parameter, and Δg_d is the difference of two Gumbel variables, while each of them is generated by $-\log \log(1/\sigma)$ with σ being a sample from uniform distribution $\text{Uniform}(0, 1)$ between 0 and 1. Theoretically, we consider

the zero temperature limit $\tau \rightarrow 0$ of Eq. 3 to obtain the binary representation, namely, $[Y_{\text{else}}]_d = 1$ with probability $[f_{\text{else},\theta}(X)]_d$ and $[Y_{\text{else}}]_d = 0$ otherwise. In practice, however, we observed that scanning the temperature from high to low multiple times helps the network to converge. q is the decoder network receiving Y_1 from the Task 1 trained network and Y_{else} from the encoder and performs the auto-encoding task for reconstructing X . $r(Y_{\text{else}}) = \prod_d (\hat{r}_d)^{[Y_{\text{else}}]_d} (1 - \hat{r}_d)^{1 - [Y_{\text{else}}]_d}$ is the Bernoulli prior distribution for p with parameters $\{\hat{r}_d\}$, which should be optimized. Note that the KL-divergence between p and r can be analytically calculated. Overall, we minimize $L(p, q, r)$ by adjusting θ that parametrizes p , q , and $\{\hat{r}_d\}$ that parametrizes r .

4.2 Step 2: New Task Training and Synthesizing Interpretation

Assume the model has internal representation $Y = \{Y_1, Y_2, \dots, Y_n, Y_{\text{else}}\}$ after learning Task 1 to n . When new Task $n+1$ is introduced, the model learns to produce Z_{n+1} that approximates labels \tilde{Z}_{n+1} using Y . Task $n+1$ interpretation synthesis can be also implemented by the IB that distils Task $n+1$ relevant information from Y as follows:

$$\max_{\theta} \left[I(\cup_{i=1}^{n,\text{else}} Y_{(i;n+1)}; Z_{n+1}) - \gamma \sum_{i=1}^{n,\text{else}} I(Y_{(i;n+1)}; Y_i) \right], Y_{(i;n+1)} = \text{Sample}[f_{(i;n+1),\theta}(Y_i)] \quad (4)$$

$Y_{(i;n+1)}$, ($i \in [1, n] \cup \text{else}$) is the information needed from Y_i to solve Task $n+1$. Again, the above sampling step is required to eliminate information irrelevant to Task $n+1$. Since $\tilde{Y}_{(i;n+1)} = \text{Sample}[f_{(i;n+1),\theta}(Y_i)]$ forms the Markov chain from Y_i to $Y_{(i;n+1)}$, together with IB, $Y_{(i;n+1)}$ is then a minimum sub-map of Y_i required for Task $n+1$. We again implement the variational IB, with lost function:

$$L(p_i, q, r_i) = \mathbb{E}_Y \left\{ \mathbb{E}_{\{Y_{(i;n+1)}\}_{i=1}^{n,\text{else}}|Y} \left[-\log q(Z_{n+1}|\{Y_{(i;n+1)}\}_{i=1}^{n,\text{else}}) \right] + \frac{\gamma}{n+1} \sum_{i=1}^{n,\text{else}} \text{KL} [p_i(Y_{(i;n+1)}|Y_i), r_i(Y_{(i;n+1)})] \right\}. \quad (5)$$

i is the index of the representation partitions. p_i is the i -th encoder network for representing the probabilistic distribution of $Y_{(i;n+1)}$ given Y_i . The d th element of $Y_{(i;n+1)}$ is sampled using the Gumbel-Softmax reparametrization trick similarly to Eq. 3 but using $f_{(i;n+1),\theta}(Y_i)$ (instead of $f_{\text{else},\theta}(X)$). q is the decoder network receiving distilled information $\{Y_{(i;n+1)}\}$ coming from all partitions ($i \in [1, n] \cup \text{else}$) to perform Task $n+1$. r_i is the prior distribution for p_i , and takes the same form as r in Eq. 2. Again, the KL-divergence between p_i and r_i can be analytically calculated.

After getting $\{Y_{(i;n+1)}\}$, the interpretation is defined as the meta-information $I(Y_{(i;n+1)}; Y_i)$ needed from each partition Y_i . We can also look into the representations of $Y_{(i;n+1)}$ to gain insight about how Task $n+1$ is solved for each example.

$Y_{(\text{else};n+1)}$ is the extra un-conceptualized information map needed to solve Task $n+1$. We can rewrite it to be Y_{n+1} and define the new un-conceptualized partition as $Y_{\text{else}'} = Y_{\text{else}} \setminus Y_{(\text{else};n+1)}$. We can then go back to Step 1 and continue the iteration for Task $n+2$ and so on.

5 The Progressive Interpretation: an Example

In this section, we demonstrate the progressive interpretation framework with an example. The CLEVR dataset is chosen in this section [23]. CLEVR dataset is a large collection of 3D rendered scenes with multiple objects with compositionally different properties. CLEVR dataset is originally designed for the visual question-answering task. For simplicity, we transfer it into a multiple-choice problem using only the pictures. Under a specific question context, the model is given a large set of four pictures and a multiple-choice answer. The model can then answer by choosing one of four unseen example pictures under the same question context without explicit language description.

In this section, we divide the tasks into two groups. Task group 1: the model is pre-trained to tell objects apart and learn to recognize part of the important properties among shape, size, color, material,

position. Task group 2: the model is asked to perform a multiple-choice task selecting a picture according to a specific question, for example, "choose the picture with red cubes," which needs information learned or not yet learned in Task 1.

5.1 Step 1: Property Learning and Information Map Splitting

We first implement Step 1 described in subsection 4.1. Before the model tries to solve the multiple-choice problem, we pre-train the model to tell different objects apart and train it to recognize certain properties. After that, the model can split the information map of each object into the trained-property related and un-related parts.

5.1.1 Image Segmentation and Property Supervised Learning

To tell objects apart, the first step we need to do is image segmentation. We implement image segmentation with Mask R-CNN [16] via fine-tuning a pre-trained Pytorch [33] Mask R-CNN on a mini-CLEVR dataset where 4000 pictures are annotated with masks [45]. The following figures show some examples of the image segmentation, and it is confirmed that the result is sufficient for the following analysis (Fig. 4).

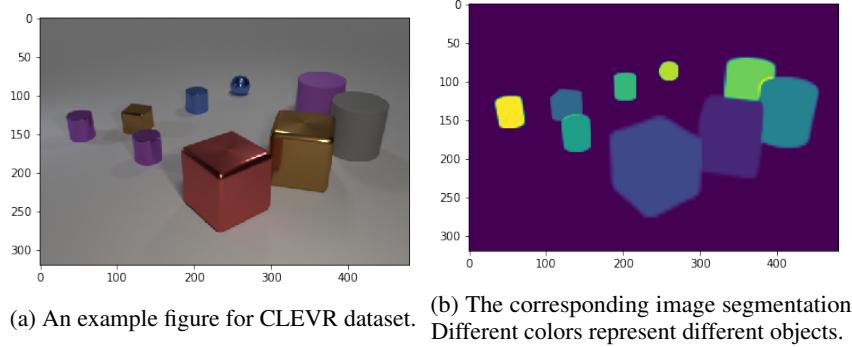


Figure 4: An image segmentation example of the CLEVR dataset.

The CLEVR dataset contains the ground truth of rendered position, color, shape, size, material of each object, which can be used for supervision to train a convolutional neural network (CNN). Since our framework is progressive, we assume that the model only has access to ground truth position, color, and material of the objects but not other properties. Following the segmentation process, the masked image of an object is sent to a Res-Net [15] and learns position, color, and material with supervision. The network output for object position is a continuous number. The root-mean-square error loss is used to quantify the position prediction. As we described in Sec. 4.1, the raw output contains a small amount of position-independent information. To eliminate it, we add Gaussian noise with a standard deviation equals to 0.2% of the image size to the network output. The size of the noise is restricted to maintain good enough precision for the position prediction. In contrast, color and material labels are categorical. The corresponding softmax outputs of the network represent the underlying probability of the one-hot categorical representation. The cross-entropy loss between the softmax outputs and the categorical labels is used for color and material prediction. Then, the internal representation for color and material is obtained by sampling from the softmax outputs. Again, this sampling step helps to eliminate task-irrelevant information encoded in the network outputs. The network is trained with loss back-propagation with the help of Pytorch's auto-grad framework. Adam is chosen as the optimizer. The model design is shown in Fig. 5. (See supplementary notes for details.)

5.1.2 Information Map Splitting by Auto-encoding

After getting the position, color, and material related information partitions, IB-induced auto-encoding can be used as the next step to extract the complementary representation Y_{else} . $f_{1-3} = \text{CNN}_{1-3}$ trained in the last-step is fixed in this step, providing information about the position, color, and material. $f_{\text{else},\theta} = \text{CNN}_{\text{else}}$ is trained to encode information other than that previously learned with the help of an IB. The scaling factor of the IB is $\gamma = 8e - 3$. Information coming from both CNN_{1-3}

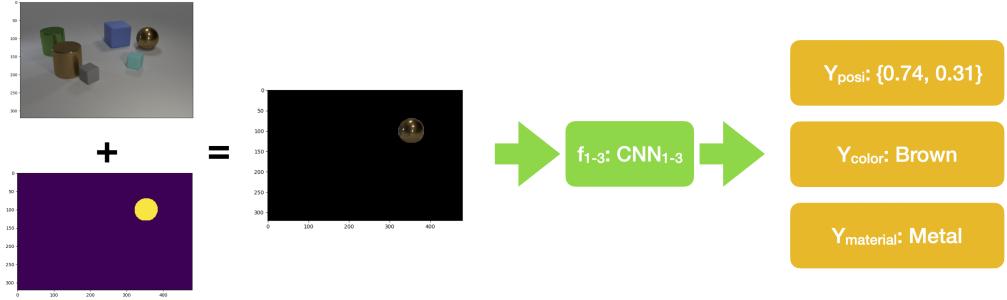


Figure 5: Property supervised learning by CNN_{1-3} .

and CNN_{else} are combined and feed into a de-convolutional neural network (DECNN) [46] to do self-prediction. Pixel-by-pixel mean-square error loss is used for self- prediction. In practice, we found out that reconstructing a cropped region where the target object is in the center instead of the original masked picture with a large background area significantly improves the auto encoding precision.

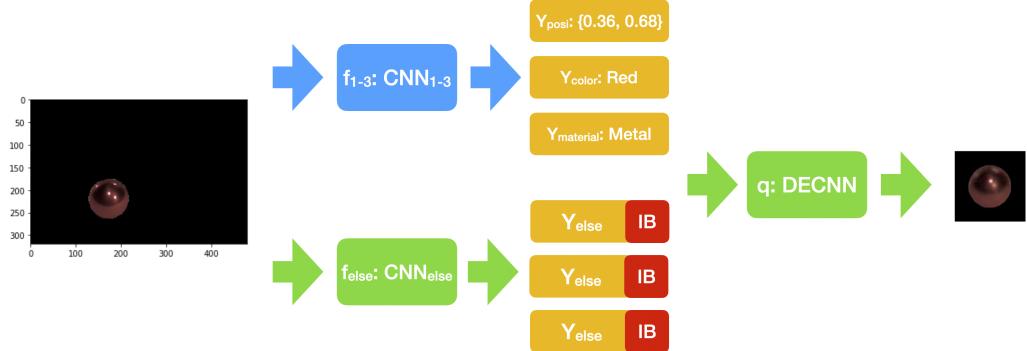


Figure 6: The computational graph of information map splitting step via auto-encoding.

After this step, we are going to have internal representation of $Y = \{Y_{\text{posi}}, Y_{\text{color}}, Y_{\text{material}}, Y_{\text{else}}\}$, where each partition represents information for the position, color, material, and other unconceptualized properties about the input. Y_{posi} is a 2D float number between 0 and 1 representing normalized X and Y position. Y_{color} is an one-hot vector with length 8, representing 8 different colors. Y_{material} is an one-hot vector with length 2, representing 2 different kinds of materials. Y_{else} is the Bernoulli distribution with dimension size 64. This internal representation will be used to solve the multiple-choice task described below and serve as the basis for the task interpretation.

5.2 Step 2: Multiple-choice Task Interpretation

In this subsection, we introduce the multiple-choice task and describe how to synthesize the interpretation of this task.

5.2.1 Task Settings

The task to be solved and interpret is a multiple-choice task regarding the categorized position (right, middle, and left), color, material, shape, and size. After choosing a certain criterion, for example: “choose the picture with a green ball,” the model is asked to pick the picture with a green ball from four candidates. To keep the task simple, we do not provide the explicit question description in natural language, and instead, we present the model with a lot of multiple-choice task examples and choice answers, and the model is supposed to find out how to solve the task without having access to the question context in natural language. Our task example generation system is designed that only

one of four pictures would satisfy the requirement. The pictures are randomly shuffled so that the probability of the choice being correct is equal to 1/4 for all four options. The following figure shows an example of the task.

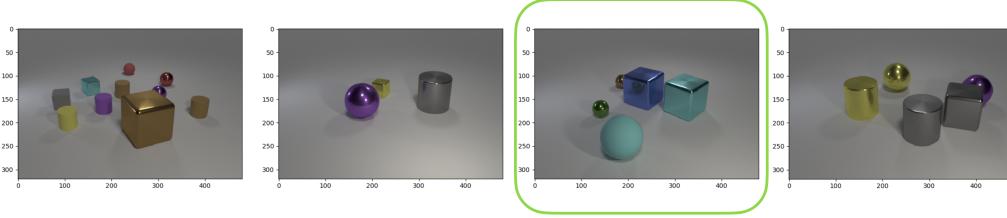


Figure 7: One example of the multiple-choice task. The model receives four pictures and is expected to output 3 for the task regarding "chose the picture with a green ball."

5.2.2 Model Setup

The CNN₁₋₃ trained in previous Step 1, which receives a masked image of an object and outputs information partition map $Y = \{Y_{\text{posi}}, Y_{\text{color}}, Y_{\text{material}}, Y_{\text{else}}\}$, per object, will be fixed in this step. Each information partition map is then feed into an IB regularized multi-layer perceptron (MLP) separately and followed by a feed-forward style neural network. The scaling factor of the IB is chosen to be $\gamma = 0.04$ for this step. The feed-forward network will first do convolution with an MLP kernel over the object dimension and followed by another MLP over four scenes to solve the multiple-choice problem. The model design for this step is shown in Fig. 8. (See supplementary notes for details.)

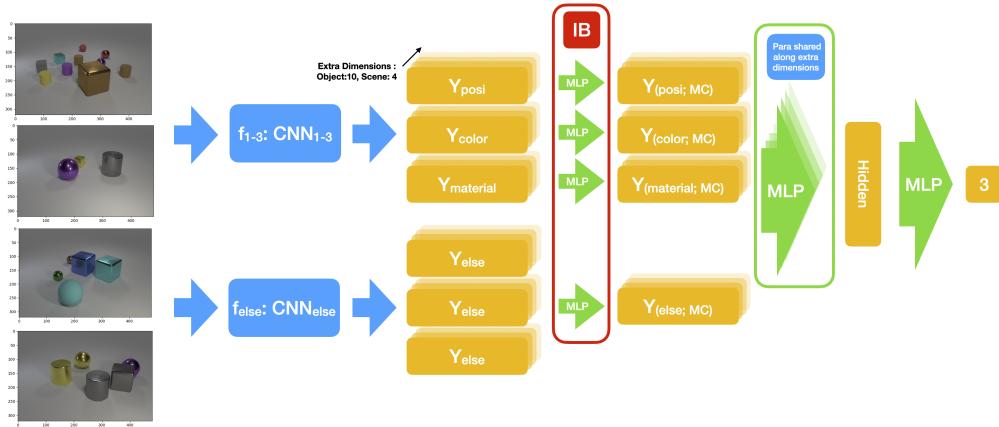


Figure 8: The computational graph of multiple-choice task learning and interpretation step. MC represents the multiple-choice task.

5.3 Experiment Result

5.3.1 Interpretation by Information Flow

The result of interpretation by information flow is shown in Table 1. The mutual information $I(Y_{(i;MC)}; Y_i)$ for $i \in \{\text{posi}, \text{color}, \text{material}, \text{else}\}$ is measured in Nat, where MC represents the multiple-choice task. Different rows represent different question types. The questions form into three groups. Group A is question 1 and 2, where information from only the previously learned part is needed. Group B contains questions 3, 4, and 5, where information from both previously learned parts and the un-conceptualized part are needed. Group C is question 6, where information from only the un-conceptualized part is needed. As expected, the model can solve the task near perfectly when all needed properties are previously learned. Moreover, it can still solve the task quite nicely, even if the un-conceptualized property is needed. Importantly, we can also interpret how the model is

Table 1: Table for Task2 interpretation, information unit (Nat/object)

Question Type	Position	Color	Material	Unknown	Correct rate
Exist Green Metal	<1E-5	0.345	0.670	<1E-5	99.1%
Left side exist Rubber	0.573	<1E-5	0.689	1.57E-03	98.0%
Exist Small Yellow Object	<1E-5	0.341	1.33E-03	0.690	99.0%
Exist Red Cube	<1E-5	0.383	2.38E-03	0.785	94.9%
Right side exist Cylinder	0.554	2.87E-04	<1E-5	0.797	94.8%
Exist Large Sphere	5.44E-03	<1E-5	<1E-5	0.289	99.3%

solving the task by calculating mutual information coming from each information map. For example, if we check the question "choose the picture with a green metal," we find out that the model actually needs 0.345 Nat of information coming from the color domain and 0.670 Nat of information from the material domain. Information coming from other domains is judged as irrelevant to this task, which is expected. If the question is "Choose the picture with a small yellow object," the model then needs 0.346 Nat of information coming from the color domain. The model also needs 0.693 Nat of information, which it has no idea what it represents since the model has not explicitly learned about size but still needs size information to solve the task. If the question is "choose the picture with a large sphere," the model finds out all previously learned properties become useless and had to pick 0.289 Nat of information from the un-conceptualized partition.

5.3.2 Single Example Interpretation and Un-conceptualized Representation

After getting the model, it is also possible to synthesize interpretation for a single example by looking into the discrete representation $Y_{(i;MC)}$ for $i \in \{\text{posi, color, material, else}\}$. Although each $Y_{(i;MC)}$ consists of multiple binary elements, here we focus on the element that has the highest mutual information with the multi-choice output for visualization. A typical example is shown in Fig. 9. This example shows the answer to the question, "choose the picture with a small yellow object." Since each multiple-choice example has four pictures, each row represents the result for each picture. The first column shows the original pictures. The second column shows the segmentation mask for the objects, where each object is colored according to the object ID. The last column shows the resulting 4-by-10 binary representation matrix distilled by the IB with each bit summarizing the corresponding $Y_{(i;MC)}$ for $i \in \{\text{posi, color, material, else}\}$. The red square represents the lower frequency ones of the binary representation, while white represents the counterparts. The dimension with size 4 represents 4 information map areas, namely position, color, material, and else. The dimension with size 10 represents each object. We can see clearly the model is trying to judge if the object has the color "yellow" while neglecting position and material information. In order to solve the problem, the model also needs information from the un-conceptualized region, and we can clearly tell that the information needed in the un-conceptualized region is actually representing the size "small." The behavior of the model is consistent with the expectation of the question regarding "small yellow object."

To examine the correctness of the information distilled from the un-conceptualized partition, we can compare it with the corresponding true label of the dataset. For example, if the question is "choose the picture with a small yellow object," we know size information is needed to answer this question, and the un-conceptualized partition should represent if the size of an object is "small." We can cross-check between the representations and the ground-truth labels by calculating their mutual information. By checking the model answering the question "choose the picture with a small yellow object," we get the mutual information between un-conceptualized partition and size "small" to be 0.662 Nat per object. By checking the question "choose the picture with a red cube," we get the mutual information between un-conceptualized partition and shape "cube" to be 0.432 Nat per object. By checking "choose the picture with a cylinder on the right side," we get the mutual information between un-conceptualized partition and shape "cylinder" to be 0.408 Nat per object.

6 Discussion

The paper proposes an information-theoretical progressive framework to synthesize interpretation. The framework is designed to satisfy some of the basic intuitions about interpretation, including

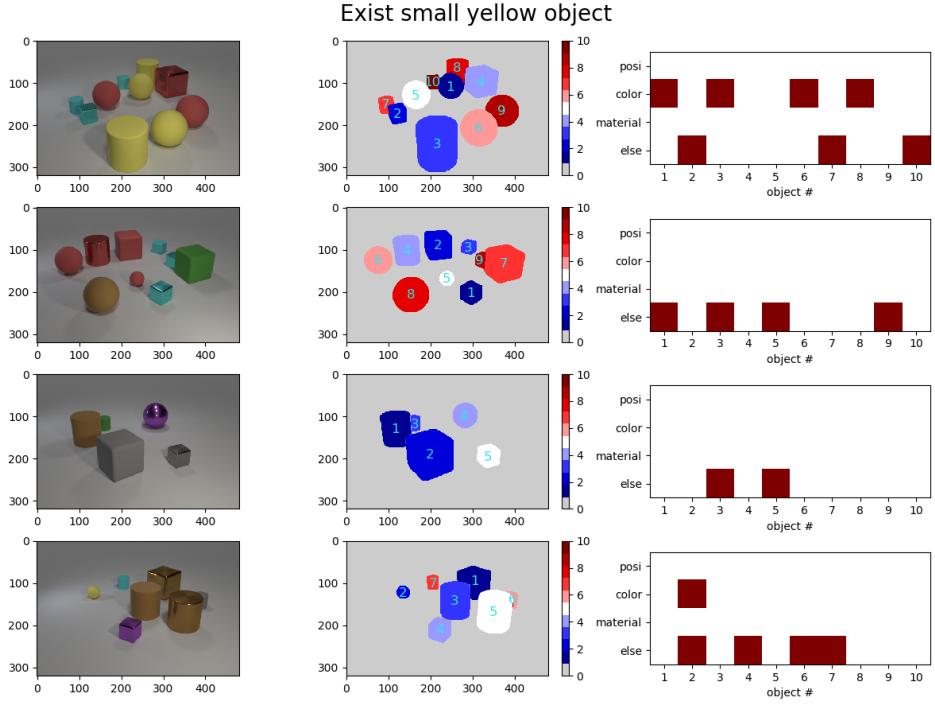


Figure 9: Single example interpretation of the question "choose the picture with a small yellow object?" The left column shows input pictures, and the middle column shows masks colored according to object IDs. We overlaid the masks with the object IDs for a visual aid. The right column shows the binary activity summarizing the distilled information layer $Y_{(i;MC)}$. The x-axis corresponds to object ID, the y-axis represents four distilled representations, namely position $Y_{(\text{posi};\text{MC})}$, color $Y_{(\text{color};\text{MC})}$, material $Y_{(\text{material};\text{MC})}$, and else $Y_{(\text{else};\text{MC})}$, where the dimension with highest mutual information is plotted. The red square represents the lower frequency realization of the binary representations, and the white represents the counterpart.

that interpretation is meta-information in nature, coarse-grained in level, involves independency, and is progressive. Changing the receiver of the interpretation from a human to a target model helps define interpretation clearly. The interpretation framework divides the input representations into independent maps according to tasks and uses the information maps to synthesize interpretation for the next task. The framework is implemented with a variational information bottleneck technique and is tested on a simplified CLEVR dataset. The framework can solve the task and synthesis non-trivial interpretation both in the form of meta-information, which summarizes necessary mutual information from split maps, and in the form of discrete representation for single-example interpretation. The framework is also shown to be able to form meaningful new representation maps progressively.

Relationship with partial information decomposition (PID). Our proposed framework shares some similarity with the PID framework [43] in the sense that both of them are trying to explain data by splitting the information map. However, the difference is also obvious. One obvious difference is that PID focuses on characterizing the data currently under consideration while our framework is progressive and learning-order dependent (see below), focusing on characterizing future data. Importantly, the number of information maps grows combinatorially with the number of neurons in the PID framework, while in our framework, the number of information splits grows linearly with tasks thanks to the training framework that actively simplifies the information map by introducing independence. On note, even though our framework tends to remove redundancy, synergy can still exist between current information splits and future tasks, which can affect the quality of synthesized interpretation.

Changes in input space. The current framework requires that input space X stays the same for all the following tasks to maximize interpretation. If X are completely different, those tasks must be solved separately. What would happen if X is slightly different for different tasks? How to handle the situation depends on the strategy. For example, if the model working on the CLEVR dataset encounters a new shape: "cone," following the current framework, the model would first classify it as a "cylinder" until the model come across some task which needs to tell apart "cone" from "cylinder." Then the model would pick some extra information from an un-conceptualized part like "sharp top" to help distinguish "cone" from "cylinder." As a result, the model would think "cone" is a sub-class of "cylinder" with "sharp top" and can further imagine a new shape like "square" with "sharp top," which is "square cone." Another example is if the distribution partially changes. Let's imagine, with the CLEVR dataset, a change where all balls suddenly become red. Under this situation, the color and shape representation still works as before. However, since once independent representation color and shape now become dependent, interpretation for the following task now has ambiguity due to the redundancy.

Relationship between interpretation quality and performance. There exists a trade-off between interpretation quality and model performance in our proposed framework. In practice, we noticed that lowering IB regularization usually results in better task performance at the cost of using more information than necessary. This leads to more redundant information partitions and an overestimation of task-relevant information. However, exchanging model performance for better understanding is not just an issue particular to our framework but is something universal. This is also the case for scientific theorems. An appropriate level of abstraction is crucial for intuitiveness and interpretability. Thus, a good balance between interpretation and performance may be the key to upgrade a model into insightful knowledge.

Relationship with the biological brain. The interpretation as a kind of meta-information is related to meta-cognition in the brain [39]. Especially the un-conceptualized information map Y_{else} is related to the meta-cognition aspect "knowing what you do not know," which is very important for the proposed interpretation framework. Brain development study also supports the idea of progressive learning, with the most famous example being the critical period hypothesis [28, 40]. Our interpretation framework is explicitly introducing independence among information maps. Meanwhile, there exist clues about the brain capable of performing independent component analysis only using local information available in each neuron [21]. Whether the brain is actively making use of this capability for task interpretation is not yet clear.

Relationship to curriculum learning. Our proposed framework said nothing about the order of tasks. In fact, no matter what the learned task sequence would be, we can always proceed with the progressive interpretation framework. However, the interpretations generated with different task sequences will be quite different from each other. Both common sense and model study shows that order of the task sequence matters [6]. It is also possible that both overall performance and accumulated interpretation quality can be a measure to guide the selection of optimum task learning order.

Our information-theoretic framework capable of forming quantifiable interpretation would inspire a shift in future research opportunities from performance-driven to understanding-driven deep learning.

7 Supplementary Notes

7.1 Network Implementation Detail

In this section, we described the detailed implementation of neural networks. Fig 10 shows the detailed topology of the convolutional network for CNN_{1-3} and CNN_{else} of Fig. 5 and Fig. 6. Detailed model shape parameters are listed in Table 2. Fig 11 shows the topology of the deconvolutional network for DECNN of Fig. 6. Detailed model shape parameters are listed in Table 3. The MLP modules in Fig. 8 are conventional multi-layer perceptrons that map the target dimension of the input tensors from a certain input size to a certain output size with several hidden layers. Each hidden layer is followed with a layer-wise normalization and a ReLU activation. Detailed shape parameters for each MLP module is shown in Table 4.

Table 2: CNN_{1–3} and CNN_{else} parameter, CNN_{else} shares the same network topology with CNN_{1–3} except for the MLP module which is shown below.

Module Name	Size [in(x,y), out(x,y)]	Channel (in, out)	Kernel	Stride	Padding
CNN _{1–3} parameter					
Conv2D1	[(480, 320), (237, 157)]	(3, 16)	7	2	0
MaxPool2D1	[(237, 157), (118, 78)]	(16, 16)	2	2	0
ResConv1	[(118, 78), (118, 78)]	(16, 16)	5	1	2
Conv2D2	[(118, 78), (114, 74)]	(16, 32)	5	1	0
MaxPool2D2	[(114, 74), (57, 37)]	(32, 32)	2	2	0
ResConv2	[(57, 37), (57, 37)]	(32, 32)	5	1	2
Conv2D3	[(57, 37), (53, 33)]	(32, 32)	5	1	0
MaxPool2D3	[(53, 33), (26, 16)]	(32, 32)	2	2	0
ResConv3	[(26, 16), (26, 16)]	(32, 32)	5	1	2
Conv2D4	[(26, 16), (22, 12)]	(32, 32)	5	1	0
MaxPool2D4	[(22, 12), (11, 6)]	(32, 32)	2	2	0
ResConv4	[(11, 6), (11, 6)]	(32, 32)	5	1	2
Linear_i2h	(2112, 128)	-	-	-	-
Linear_h1	(128, 64)	-	-	-	-
Linear_h2o	(64, 12)	-	-	-	-
CNN _{else} parameter					
Linear_i2h	(2112, 512)	-	-	-	-
Linear_h1	(512, 256)	-	-	-	-
Linear_h2o	(256, 128)	-	-	-	-

Table 3: DECNN parameter, note that the images which DECNN works with has equal x and y sizes.

Module Name	Size (in, out)	Channel (in, out)	Kernel	Stride	Padding
Linear_i2h	(140, 256)	-	-	-	-
Linear_h1	(256, 512)	-	-	-	-
Linear_h2o	(512, 1152)	-	-	-	-
ResConv1	(6, 6)	(32, 32)	5	1	2
ConvTranspose2D1_1	(6, 12)	(32, 32)	2	2	0
ConvTranspose2D1_2	(12, 16)	(32, 32)	5	1	0
ResConv2	(16, 16)	(32, 32)	5	1	2
ConvTranspose2D2_1	(16, 32)	(32, 16)	2	2	0
ConvTranspose2D2_2	(32, 36)	(16, 16)	5	1	0
ResConv3	(36, 36)	(16, 16)	5	1	2
ConvTranspose2D3_1	(36, 72)	(16, 16)	2	2	0
ConvTranspose2D3_2	(72, 147)	(16, 3)	5	2	0

Table 4: MLP module parameters for multiple-choice tasks, x size equals y size. b stands for batch size. "Target dim#" stands for target number of dimension the MLP is going to map from.

Module Name	Input data shape	Target dim#	Input size	Output size	Hidden size
MLP: Y_{posi}	(b, 4, 10, 2)	4	2	8	(16, 16)
MLP: Y_{color}	(b, 4, 10, 8)	4	8	8	(16, 16)
MLP: Y_{material}	(b, 4, 10, 8)	4	2	8	(16, 16)
MLP: Y_{else}	(b, 4, 10, 64)	4	64	16	(32, 32)
MLP: Y to hidden	(b, 4, 10, 40)	4	40	1	(32, 16, 8)
MLP:hidden to out	(b, 4, 10)	3	10	1	(5)

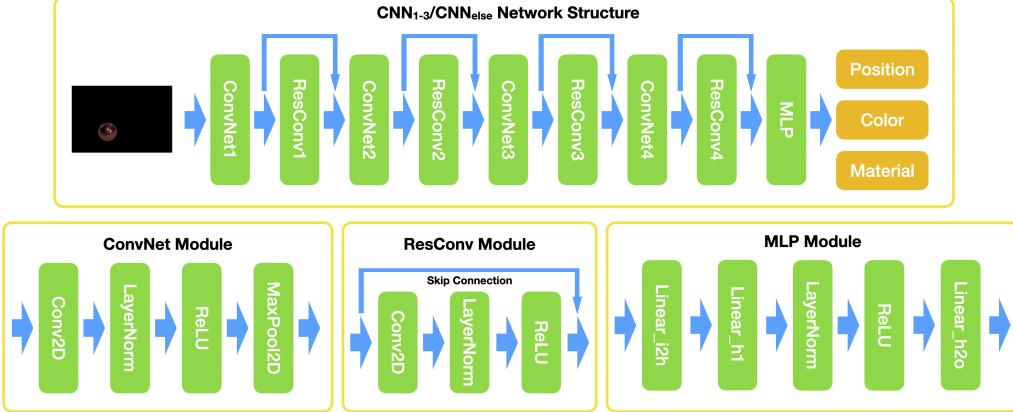


Figure 10: Network topology for CNN_{1-3} and CNN_{else}

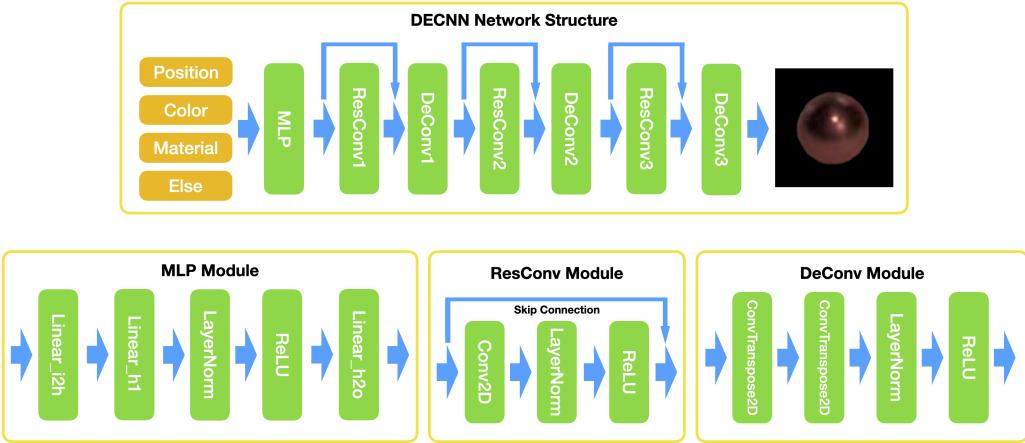


Figure 11: Network topology for DECNN

7.2 Other Training Details

Temperature Schedule for Gumbel Softmax: As mentioned in Sec. 4.1, instead of fixing the temperature in Gumbel softmax at a constant low temperature, we found out that multiple scans of the temperature from high to low benefits training. We use an exponential schedule to control the Gumbel softmax temperature $\tau = \exp(-5(n \times s - \lfloor n \times s \rfloor))$ where n is the total number of scans, and s is the training schedule that starts with 0 and ends with 1.

Learning Rate Schedule: We implement a standard plateau-and-decay strategy for learning rate schedule. We set three stages of the learning rate, namely, 1e-4, 1e-5, and 2e-6. For each stage of the learning rate, we train the model until reaching a plateau where the lost function doesn't decrease any further, and then we decrease the learning rate to the next stage. The number of epochs needed to reach a plateau depends on different tasks. For the supervised learning task, the model usually needs several tens of epochs to reach the plateau, while for the auto-encoding task, the needed number of epochs can be several hundred, with each epoch contains 70K training examples. For the multiple-choice task, the needed number of epochs is around one hundred, with each epoch contains 100K examples.

IB scaling factor Schedule: The work [35] claims that training a deep network usually consists of two phases: training label fitting phase and information compression phase. Inspired by this work, we add a warm-up training phase where IB scaling factor is set to zero and use learning rate 1e-4 to train the network. After that, the IB scaling factor is set back to normal, and information starts to get compressed. This strategy especially works well with the multiple-choice task, where we encountered

some cases where the loss function never goes down if we start training with a non-zero IB scaling factor.

7.3 Code Availability

Source code for this project can be found at github:

https://github.com/hezq06/progressive_interpretation

7.4 Author contributions

Z.H. and T.T. planned the project and built the theoretical framework. Z.H. performed the simulations. Z.H. and T.T. wrote the manuscript.

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