CONCEPT GRADIENT: CONCEPT-BASED INTERPRETATION WITHOUT LINEAR ASSUMPTION

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ABSTRACT

Concept-based interpretations of black-box models are often more intuitive for humans to understand. The most widely adopted approach for concept-based, gradient interpretation is Concept Activation Vector (CAV). CAV relies on learning a linear relation between some latent representation of a given model and concepts. The premise of meaningful concepts lying in a linear subspace of model layers is usually implicitly assumed but does not hold true in general. In this work we proposed Concept Gradient (CG), which extends concept-based, gradient interpretation methods to non-linear concept functions. We showed that for a general (potentially non-linear) concept, we can mathematically measure how a small change of concept affects the model's prediction, which is an extension of gradient-based interpretation to the concept space. We demonstrated empirically that CG outperforms CAV in attributing concept importance on real world datasets and performed a case study on a medical dataset.

1 INTRODUCTION

Explaining the prediction mechanism of machine learning models is important, not only for debugging and gaining trust, but also for humans to learn and actively interact with them. Many feature attribution methods have been developed to attribute importance to input features for the prediction of a model (Sundararajan et al., 2017; Zeiler & Fergus, 2014). However, input feature attribution may not be ideal in the case where the input features themselves are not intuitive for humans to understand. It is then desirable to generate explanations with human-understandable concepts instead, motivating the need of **concept based explanation**. For instance, to understand a machine learning model that takes microscopy images as input and predicts the underlying gene expression, attributing importance to high-level concepts such as morphological features of cells explains the predictions better than to raw pixel values.

The most popular approach for concept-based interpretation is Concept Activation Vector (CAV) Kim et al. (2018). CAV represents a concept with a vector in some layer of the target model and evaluates the sensitivity of the target model's gradient in the concept vector's direction. Many followup works are based on CAV and share the same fundamental assumption that concepts can be represented as a linear function in some layer of the target model (Ghorbani et al., 2019; Schrouff et al., 2021). However, this assumption generally does not hold, and such restriction limits the application of concept-based attribution to relatively simple concepts.

In this paper, we rethink the problem of concept-based explanation and tackle the fundamental linear separability issue. One perspective of model interpretation is to measure how small perturbations to a feature affect the prediction, which can be measured by the input gradients in typical feature-based explanations. A question naturally arises: is it possible to extend the notion of the gradient to the concept space? If so, non-linear concepts can be easily handled without additional assumptions. In this paper, we answer this question in affirmative and provide a simple formulation of Concept Gradient (CG), which measures how small changes of concept affect the model's prediction mathematically. If a unique function from concept to prediction exists, CG exactly recovers the gradient of that function. Otherwise, though there exist an infinite number of functions that map concept to prediction, there is a unique mapping that has minimal changes in the input space, and CG will capture the gradient of such function. Given any model f and (potentially non-linear) concept g, CG simply computes the gradient to linearize both functions at individual input points to capture

local linear behavior of the joint function. We discovered that when the concept function is linear, CG recovers CAV (with a slightly different scaling factor), which explains why CAV works well in linearly separable cases. The derivation and formulation of CG also provide insight into understanding how concept functions and models interact locally. We showed in real world datasets that the linear separability assumption of CAV does not always hold and CG outperforms CAV consistently. The average best local recall@30 of CG is higher than the best of CAV by 7.9%, while the global recall@30 is higher by 21.7%.

2 PRELIMINARIES

Problem definition In this paper we use $f : \mathbb{R}^d \to \mathbb{R}^k$ to denote the machine learning model to be explained, $x \in \mathbb{R}^d$ to denote input, and $y \in \mathbb{R}^k$ to denote the label. For an input sample $\hat{x} \in \mathbb{R}^d$, concept-based explanation aims to explain the prediction $f(\hat{x})$ based on a set of m concepts $\{c_1, \ldots, c_m\}$. In particular, the goal is to reveal how important is each concept to the prediction. Concepts can be given in different ways, but in the most general forms, we can consider concepts as functions mapping from the input space to the concept space, denoted as $g_i : \mathbb{R}^d \to \mathbb{R}$ for each concept i. The function can be explicit or implicit. For example, morphological features such as cell perimeter and circularity can be given as explicit functions designed by domain experts. On the other hand, many concept-based explanations in the literature consider concepts given as a set of examples, which are finite observations from the underlying concept function. We further assume f and g are differentiable which follows the standard assumption of gradient-based explanation methods.

For simplicity we represent all g_i together as a joint function $g : \mathbb{R}^d \to \mathbb{R}^m$ mapping input to an m-dimensional concept space. We denote a vector in the concept space as $c \in \mathbb{R}^m$ and $\hat{c} = g(\hat{x})$ is the concept vector for a given instance. For each concept function g_i, we can define a local concept relevance score $R_{\hat{x}}(i, j)$ to represent how concept $\hat{c}_i$ affects target class prediction $\hat{y}_j = f_j(\hat{x})$. Further, by aggregating over all the input instances $\{x_1, \cdots, x_n\}$, we can define a global concept relevance score $R(i, j)$ to represent how a concept g_i affects the target class prediction y_j. The goal is to calculate concept relevance scores such that the scores reflect the true underlying concept importance, possibly aligned with human intuition.

Recap of Concept Activation Vector (CAV) Concept activation vector is a concept-based interpretation method proposed by Kim, et al. (Kim et al., 2018). The idea is to represent a concept with a (concept activation) vector and evaluate the alignment between the input gradients of the target model and the vector. In order for the concept to be represented well by a vector, the concept labels must be linearly separable in the space where the vector lies. The authors implicitly assumed that there exists a layer in the target model where concept labels can be linearly separated.

Let $\boldsymbol{v}_c$ denote the concept activation vector associated with concept c. The authors define the conceptual sensitivity score to measure concept importance

$$S_f(x) := \nabla f(x) \cdot (\boldsymbol{v}_c / \|\boldsymbol{v}_c\|). \tag{1}$$

The main caveat with the conceptual sensitivity scores is that the underlying concept function is not guaranteed to lie in the linear subspace of some neural activation space. Attempting to fit the concept function with a linear model likely leads to poor results for non-trivial concepts, leading to inaccurate conceptual sensitivity scores.

3 PROPOSED METHOD

3.1 DEFINITION OF CONCEPT GRADIENT (CG)

We assume x is the input instance, $y = f(x)$ is the k-dimensional model output and $c = g(x)$ is the m-dimensional concepts. For standard feature-based explanation, which aims to measure the importance of each input dimension of x, gradient-based methods have been widely used. The gradient map $\nabla f(x)$ measures how small changes on each input dimension affect the output and serves as the foundation of many existing explanation methods (Ancona et al., 2017; Shrikumar et al., 2017; Sundararajan et al., 2017). This paper is the first formally extending the notion of gradient to

concept-based explanation, and by doing so we enable explanation of any general nonlinear concept. We define the **Concept Gradient** (CG) to measure how small perturbations on each concept affect the label prediction:

$$\text{(General version of CG)} \quad \text{CG}(x) := \nabla g(x)^{\dagger} \nabla f(x). \tag{2}$$

Note that when computing the gradient of a multivariate function such as f, we follow the convention that $\nabla f(x) \in \mathbb{R}^{d \times k}$ where the $(\nabla f(x))_{ij} = \frac{\partial f_j(x)}{\partial x_i}$. And $\nabla g(x)^{\dagger} \in \mathbb{R}^{m \times d}$ is the pseudo-inverse of $\nabla g(x)$. CG(x) will thus be an $m \times k$ matrix and its (i, j) element measures the contribution of concept i to label j. Pseudo-inverse is a generalized version of matrix inversion—when the inverse does not exist, it forms the (unique) inverse mapping from the column space to the row space of the original matrix, while leaving all the other spaces untouched. Although multiple inverse matrix options exist when g is invertible, using pseudo-inverse prevents mis-attribution of importance from other spaces irrelevant to $\nabla g(x)$.

Similar to CAV, CG can be computed at any layer of a neural network by setting x as the neurons in a particular layer. In practice, CG can be easily computed given access to a concept prediction model g. The concept model can also be trained from representative concept data samples. More details regarding the implementation of CG in practice can be found in Section 3.5.

Before formally deriving CG, we use a few special cases to illustrate the method. First, for the case when x, y and c are all scalars ($k = m = d = 1$), there exists a function mapping c to y locally around a particular $\hat{c} = g(\hat{x})$ as long as $g'(\hat{x}) \neq 0$. Basic on calculus, under this condition in 1D case we have $\frac{dc}{dx} = 1/(\frac{dx}{dc})$ at $\hat{x}$, so concept gradient exactly recovers $\frac{dy}{dc}$:

$$\frac{dy}{dc}\Big|_{c=\hat{c}} = \frac{dy}{dx}\Big|_{x=\hat{x}} \cdot \frac{dx}{dc}\Big|_{c=\hat{c}} = \frac{dy}{dx}\Big|_{x=\hat{x}} (\frac{dc}{dx}\Big|_{x=\hat{x}})^{-1} = f'(\hat{x}) \cdot \frac{1}{g'(\hat{x})} = \text{CG}(\hat{x}). \tag{3}$$

This can be easily extended to the case when $m = d$ and $\nabla g(\hat{x})$ is invertible. In this case, there exists an unique function $g^{-1}(c)$ mapping c to x locally around $\hat{c}$, and by the chain rule we show CG$(\hat{x})$ is equivalent to the derivative of y with respect to c:

$$\frac{\partial y}{\partial c}\Big|_{c=\hat{c}} = \frac{\partial f(g^{-1}(c))}{\partial c}\Big|_{c=\hat{c}} = \nabla g^{-1}(\hat{c}) \nabla f(g^{-1}(\hat{c})) = (\nabla g(\hat{c}))^{-1} \nabla f(\hat{x}) = \text{CG}(\hat{x}).$$

The pseudo-inverse in (2) extends this derivation to the general case when m, d are in arbitrary dimensions, and we will formally derive it in Section 3.4.

3.2 CG FOR A SINGLE CONCEPT

In previous concept attribution methods such as CAV, a canonical setting is to measure the importance of a single concept. Here we try to simplify CG in this setting when concepts are scalars and discuss the relationship with CAV.

When $m = 1$, $\nabla g(x)$ is a $d \times 1$ vector and by the definition of pseudo-inverse, $\nabla g(x)^{\dagger} = \frac{\nabla g(x)^T}{\|\nabla g(x)\|^2}$, which leads to the following simplified concept gradient when explaining a single concept:

$$\text{(Single-concept CG)} \quad \text{CG}(x) = \left(\frac{1}{\|\nabla g(x)\|^2} \nabla g(x)^T \right) \nabla f(x) = \frac{1}{\|\nabla g(x)\|^2} \nabla g(x)^T \nabla f(x). \tag{4}$$

In this case, CG is simply a normalized version of the inner product between the gradient of concept ($\nabla g(x)$) and the gradient of the prediction model ($\nabla f(x)$). This is the main formulation we are going to use in practice, since we found applying CG to each concept individually will match better with human perception, as will be discussed in Section 3.3.

In the special case when $g(x) = v_C \cdot x$ is a linear function (the assumption of CAV), we have CG$(x) = v_C^T \nabla f(x) / \|v_C\|^2$, which is almost identical to conceptual sensitivity score in Eq 1 except a slightly different normalization term where CAV normalizes the inner product by $1/\|v_C\|$. Furthermore, the sign of CG and CAV will be identical which explains why CAV is capable of retrieving important concepts under the linearly separable case.

Here we use a simple example to demonstrate that the normalization term could be important in some special cases. Consider f as the following network with two-dimensional input $[x_0, x_1]$:

$$y = 0.1 z_0 + z_1, \begin{bmatrix} z_0 \\ z_1 \end{bmatrix} = \begin{bmatrix} 100 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} h_0 \\ h_1 \end{bmatrix}, \begin{bmatrix} h_0 \\ h_1 \end{bmatrix} = \begin{bmatrix} 0.01 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} x_0 \\ x_1 \end{bmatrix}, \tag{5}$$

and $c_0 = x_0$, $c_1 = x_1$. Then we know since $y = 0.1z_0 + z_1 = 0.1x_0 + x_1$, the contribution of c_1 should be 10 times larger than c_0. In fact, $\frac{dy}{dc_0} = 0.1$, $\frac{dy}{dc_1} = 1$ and it's easy to verify that CG will correctly obtain the gradient no matter which layer is chosen for computing (4). However, the results will be wrong when a different normalization term is used when computing concept explanation on the hidden layer h. Since $c_0 = 100h_0, c_1 = h_1, y = 10h_0 + h_1$, we have

$$\begin{aligned}
&\text{For concept } c_0\text{: } v = \frac{dc_0}{dh} = [100, 0]^T, u = \frac{dy}{dh} = [10, 1], v^T u/\|v\| = 10, v^T u/\|v\|^2 = 0.1 \\
&\text{For concept } c_1\text{: } v = \frac{dc_1}{dh} = [0, 1]^T, \frac{dy}{dh} = [10, 1], v^T u/\|v\| = 1, v^T u/\|v\|^2 = 1.
\end{aligned} \tag{6}$$

Therefore, the normalization term used in CAV (in red color) will lead to a conclusion that $c_0 > c_1$, while CG (in blue color) will correctly get the actual gradient and conclude $c_1 > c_0$. This is mainly because CG is formally derived from the actual gradient, as we will discuss below. In contrast, CAV is based on the intuition of "gradient sensitivity" and not the exact chain-rule gradient, so is subject to per-dimension scaling.

Although the normalization term can be important in some special cases, in practice we do not find the attribution results to be much different with different normalization terms, probably because such extreme per-dimensional scaling rarely happens in well-trained neural networks. We compared different methods of calculating CG (including different normalization schemes) empirically in Section 4.1. Thus, in practice if the concept can be accurately modeled by a linear function, CAV is capable of retrieving the concept gradient. However, in general the linear separability assumption does not hold and CG can handle any nonlinear concept.

3.3 Should we explain multiple concepts jointly or individually?

When attributing the prediction to multiple concepts, our flexible framework enables two options: 1) treating each concept independently using single-concept attribution formulation (4) 2) Combining all the concepts together into $c \in \mathbb{R}^m$ and run CG. Intuitively, option 2 takes the correlations between concepts into account while option 1 does not. When both concepts A and B are important for prediction but concept A is slightly more important than concept B, option 1 will identify both of them to be important while option 2 may attribute the prediction to concept B only. For example, when $y = x_0 + x_1, c_0 = x_0, c_1 = x_0 + 0.1x_1$, option 1 will identify both concepts to be important, while option 2 will produce negative score for c_0. Details can be found in the appendix. We further compared these two options on real datasets. The results are presented in Section 4.1. We verified that empirically applying pseudo-inverse individually for each concept is better aligned with the attributes labeled by humans.

3.4 Deriving CG

Here we derive CG in the general case when $\nabla g(x)$ is not invertible. For simplicity, we assume $\nabla g(x)$ has full column rank, which implies g is surjective (this is always true when $m = 1$). Otherwise we can directly constrain c within the row space of $\nabla g(x)$ and the arguments below will still go through.

Our goal is to construct a mapping from c to x and analyze the gradient. However, there are infinitely many functions from c to x that can locally inverse $g(x)$ since the dimension of concept (m) could be much smaller than input dimension d. Despite an infinite number of choices, we show the gradient of such function always follows a particular form:

Theorem 1. *Consider a particular point $\hat{x}$ with $\hat{c} = g(\hat{x})$. Let $h : \mathbb{R}^m \to \mathbb{R}^d$ be a smooth and differentiable function mapping c to x and satisfy $g(h(c)) = c$ locally within the ϵ-ball around $\hat{c}$, then the gradient of h will take the form of*

$$\nabla h(\hat{c}) = \nabla g(\hat{x})^{\dagger} + G_{\perp}, \tag{7}$$

where any row vector of $G_{\perp}$ belongs to null$(\nabla g(x_0)^T)$ (null space of $\nabla g(x_0)^T$).

The proof of the theorem is deferred to the appendix. Intuitively, this implies the gradient of h will take a particular form in the space of $\nabla g(x)^T$ while being arbitrary in its null space since any change

in the null space cannot locally affect c. We can verify that $g(x)$ is locally unchanged in the null space of $\nabla g(x)^T$, as

$$g(x + G_\perp) \approx g(x) + \nabla g(x)^T G_\perp = g(x).$$

This is saying there are multiple choices in Δx to achieve the same effect on c, since any additional perturbation in null$(\nabla g(x)^T)$ won't make any change to c locally. For example, when we want to change the concept of "color" in an image by Δx, we can have Δx only including the minimal change (e.g., only changing the color), or have Δx including change of color and any arbitrary change to another orthogonal factor (e.g., shape). For concept-based attribution, it is natural to consider the minimal space of x that can cover c, which corresponds to setting $G_\perp$ as 0 in (7).

If we pick such h then $\nabla h(\hat{c}) = \nabla g(\hat{x})^\dagger$, so we can represent y as a function of c locally by $y = p(c) := f(h(c))$ near $\hat{c}$. By chain rule we then have

$$\nabla p(\hat{c}) = \nabla h(\hat{c}) \nabla f(\hat{x}) = \nabla g(\hat{x})^\dagger \nabla f(\hat{x}) = \text{CG}(\hat{x}).$$

In summary, although there are infinitely many functions from c to y since the input space has a larger dimension than the concept space, if we consider a subspace in x such that change of x will affect c (locally) and ignore the orthogonal space that is irrelevant to c, then any function mapping from c to y through this space will have gradient equal to Concept Gradient defined in (2).

3.5 Implementation of CG

Implementing CG is rather simple in practice. Given a target model f to interpret, CG can be calculated if a concept model g is also given by the user. Generally, any concept model g sharing the same input representation as f would suffice. It is also possible to train a concept model given pairs of data samples representing the concepts. Empirically, we discovered that training g by freezing some layers of f and finetuning it to predict concept labels yields the best performance. The similarity between the two models leads to similar utilization of input representation, which benefits importance attribution via gradients.

Analogous to conceptual sensitivity and TCAV score, CG can also evaluate per-sample or per-class concept importance when interpreting classification models. For each data sample, the input gradients for both f and g can be easily and efficiently evaluated with automatic differentiation packages. We can calculate its concept gradient via Eq 2, which we will refer to as "local CG" for clarity. Local CG can be aggregated over samples in the same class to obtain the per-class concept importance, which will be referred to as "global CG". Following TCAV (Kim et al., 2018), we evaluated global CG by calculating the proportion of positive local CG over a set of data samples of the same class $\mathcal{Z}_y = \{(x_1, y), \dots (x_n, y)\}$.

$$\text{global CG}(\mathcal{Z}_y) = \frac{|\{(x, y) \in \mathcal{Z}_y : \text{local CG}(x) > 0\}|}{|\mathcal{Z}_y|}$$

Global CG can also be aggregated differently, suitable to the specific use case.

4 Experimental Results

We benchmarked CG on real world datasets with ground-truth concept labels to show that CG outperforms CAV in accurately attributing concept importance. We then presented qualitative results as well as a case study on critical domain applications.

4.1 Quantitative analysis

In this experiment, our goal is to quantitatively benchmark how well CG is capable of correctly retrieving relevant concepts in a setting where the ground truth concept importance is available. In this case, the ground truth concept importance consists of human annotations of how relevant a concept is to the model prediction. We can evaluate the quality of concept importance attribution by treating the task as a retrieval problem. Specifically given a data sample and its target class prediction, the concept importance given by CG is used to retrieve the most relevant concepts to the prediction. A good importance attribution method should assign highest concept importance to concepts relevant to the class.

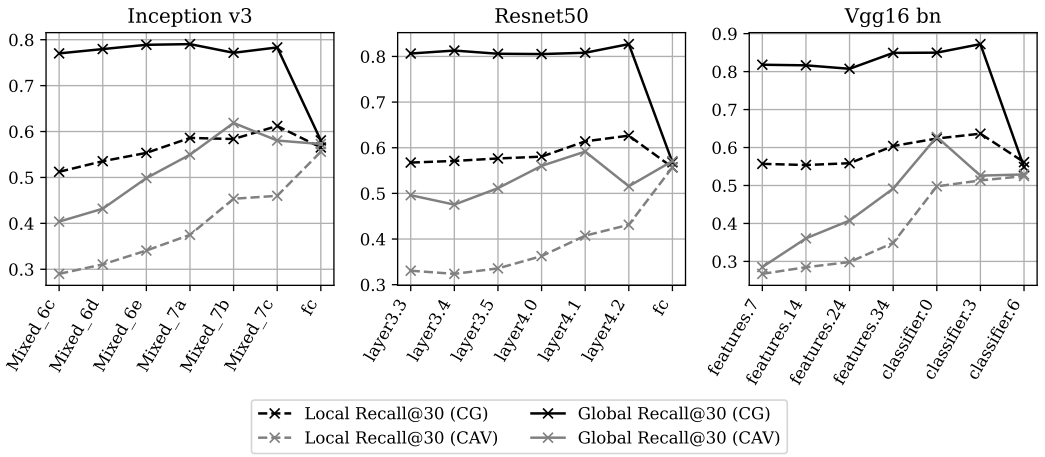

Figure 1: CUB concept recalls for different input representations in various layers and architectures (left to right, deep to shallow layers). CG consistently performs better than CAV locally and globally.

We benchmarked local (per-sample) and global (per-class) concept importance attribution separately. Given an input sample (x_i, y_i), its ground truth relevant concept set $\hat{C}_i$ and the top k attributed local important concept set C_i, the local recall@k is defined as

$$\text{Local Recall@k} := \frac{|\hat{C}_i \cap C_i|}{k}$$

Given a set of data samples from the same class $\mathcal{Z}_y = \{(x_1, y), \ldots, (x_n, y)\}$ and their ground truth relevant concept sets $\{\hat{C}_1, \ldots, \hat{C}_n\}$, we can obtain the class-wise ground truth concept set $\hat{C}_y$ by majority voting. We can also obtain the top k attributed global important concept set C_y. The global recall@k is then defined as

$$\text{Global Recall@k} := \frac{|\hat{C}_y \cap C_y|}{k}$$

The local attribution performance is measured by the average local recall@k (over samples) on a holdout testing set. The global attribution performance is measured by the average global recall@k (over classes) on a holdout testing set.

Dataset. We experimented on CUB-200-2011 (Wah et al., 2011), a dataset for fine-grained bird image classification. It consists of 11k bird images, 200 bird classes, and 312 binary attributes. These attributes are descriptors of bird parts (e.g. bill shape, breast pattern, eye color) that can be used for classification. We followed experimental setting and preprocessing in (Koh et al., 2020) where attributes with few samples are filtered out leaving 112 attributes as concepts for interpretation.

Evaluation. For CG, we finetuned the target model f for fine-grained bird classification on the concept labels to obtain the concept model g. We also evaluated CAV on the corresponding model layers for comparison. All the details regarding model training for reproducibility can be found in Appendix I.2. The local and global recalls for all models and layers are plotted in Fig 1. The layers in the x-axis are shallow to deep from left to right.

Tables 1 and 2 compares the best result of CAV and CG of the three different model architectures. CG consistently outperforms CAV in concept importance attribution (recall) since the non-linearity in CG captures concepts better (higher concept accuracy).

Ablation study on model layers. We performed an ablation study on performing attribution with different input representations, as given by different model layers. We observe that for every input representation in every model, CG consistently outperforms CAV in concept importance attribution, both locally and globally. For CG, the performance trend peaks in the penultimate layer representation. While finetuning more layers may lead to better concept prediction, it does not necessarily translate into better attribution. There is a trade-off between the concept model g capturing the concept well (finetuning more layers better) and utilizing the input more similarly to the target model f (finetuning less layers better). In this case, the input representation in the penultimate layer retains

Table 1: Local concept importance attribution comparison on CUB

Model	Method	Concept Accuracy	Local (per-sample)		
			R@30	R@40	R@50
Inception v3	CAV	0.709	0.556	0.664	0.745
	local-CG	0.791	0.612	0.718	0.790
Resnet50	CAV	0.727	0.557	0.663	0.740
	local-CG	0.793	0.627	0.726	0.794
Vgg16 bn	CAV	0.703	0.525	0.628	0.708
	local-CG	0.793	0.637	0.733	0.800

Table 2: Global concept importance attribution comparison on CUB

Model	Method	Concept Accuracy	Global (per-class)		
			R@30	R@40	R@50
Inception v3	TCAV	0.709	0.619	0.742	0.822
	global-CG	0.791	0.790	0.894	0.944
Resnet50	TCAV	0.727	0.592	0.692	0.775
	global-CG	0.793	0.827	0.915	0.951
Vgg16 bn	TCAV	0.703	0.628	0.747	0.832
	global-CG	0.793	0.872	0.935	0.961

sufficient information to capture the concept labels. For CAV, the performance is generally better in deeper layers since concepts are more linearly separable in the latter layers. Unlike the non-linearity of CG, CAV is unable to exploit the more concept information contained in the representation of earlier layers.

Ablation study on pseudo-invsere calculation. We compared different methods of calculating the concept gradient, including pseudo-inverse jointly with all concepts versus each concept separately as well as various gradient normalization schemes. We ran all experiments on Inception v3 with finetuned layers `Mixed_7b+`. The results are presented in Table 3. Joint represents the pseudo-inverse being performed on all the concepts jointly while individual represents the pseudo-inverse being performed on each individual concept separately. Un-normalized represents pure inner product between $\nabla f(x)$ and $\nabla g(x)$ without normalization, normed $\nabla g(x)$ with normalized $\nabla g(x)$, and cosine with both normalized $\nabla f(x)$ and $\nabla g(x)$. Recall that individual pseudo-inverse is exactly inner product normalized with squared concept norm. We observe that the concept attribution with joint pseudo-inverse is not aligned with human perception of concept importance while all other methods performs equally well. This supports the argument that the gradient norms in trained neural network are well-behaved and it is unlikely to encounter cases where normalization influences the attribution results significantly.

Table 3: Comparison of different CG pseudo-inverse calculations

Method		Local			Global		
		R@30	R@40	R@50	R@30	R@40	R@50
Pseudo-inverse	Joint	0.3449	0.4399	0.5295	0.4091	0.5107	0.6072
	Independent	0.6121	0.7175	0.7896	0.7832	0.9071	0.9492
Inner Product	Un-normalized	0.6009	0.7176	0.8013	0.7832	0.9071	0.9492
	Normed $\nabla g(x)$	0.6104	0.7196	0.7985	0.7832	0.9071	0.9492
	Cosine Similarity	0.6104	0.7196	0.7985	0.7832	0.9071	0.9492

4.2 Qualitative analysis

The purpose of this experiment is to provide intuition and serve as a sanity check by visualizing instances and how CG works.

Dataset. We conducted the experiment on the Animals with Attributes 2 (AwA2) dataset (Xian et al., 2018), an image classification dataset with 37k animal images, 50 animal classes, and 85 binary attributes for each class. These concepts cover a wide range of semantics, from low-level colors and textures, to high-level abstract descriptions (e.g. “smart”, “domestic”). We further filtered out 60 concepts that are visible in the input images to perform interpretation.

Figure 2: Visualization of instances with highest CG attributed importance (AwA2 validation set) for each concept (top 1 instance in the top 3 classes per concept). CG is capable of handling low level (colors), middle level (textures), and high level (body components) concepts simultaneously.

Evaluation. The evaluation is performed on the validation set. Fig 2 visualizes the instances with the highest CG importance attribution for 6 selected concepts, filtering out samples from the same class (top 1 instance in the top 3 classes). The concepts are selected to represent different levels of semantics. The top row contains colors (low-level), the middle row contains textures (medium-level), and the bottom row contains body components (high-level). Observe that CG is capable of handling different levels of semantics simultaneously well, owing to the expressiveness of non-linear concept model g. Additionally, we presented randomly sampled instances from the validation set and listed top-10 most important concepts as attributed by CG (see the appendix). We intentionally avoided curating the visualization samples to demonstrate the true importance attribution performance of CG. The most important concepts for each instance passed the sanity check. There are no contradictory concept-class pairings and importance is attributed to concepts existent in the images.

4.3 Case study on mortality risk of myocardial infarction complications

The purpose of the case study is to demonstrate the effectiveness of CG in critical domain applications beyond classification tasks on natural-image data.

Dataset. We experimented on the Myocardial infarction complications database. The database consists of 1,700 entries of patient data with 112 fields of input tabular features, 11 complication fields for prediction, and 1 field of lethal outcome also for prediction. The input features are measurements taken when the patients were admitted to the hospital due to myocardial infarction as well as past medical records. The target models predict lethal outcome given the 112 input fields. The concept models predict the complications given the same 112 input fields.

Evaluation. Our goal is to interpret the lethal outcome with the complications and compare our interpretation with existing literature regarding how each complication affects the risk of death. We expect good interpretations to assign high relevance to complications that pose high mortality risk. Table 4 shows the global CG scores (aggregated by averaging local CG) as well as the excerpted description of the complication mortality risk in the existing medical literature. The severity of descriptions in the medical literature is largely aligned with the CG scores. The highest risk complications are attributed the most importance (e.g. relapse of MI) while the lower risk complications are attributed the least importance (e.g. post-infarction angina). This supports CG as an effective method for real-life practical use for interpreting models in critical domains. We also provided TCAV scores (aggregated by averaging local CAV) for comparison, which is largely aligned with CG with few exceptions (e.g. chronic heart failure) where the CAV interpretation deviate from literature. The full table can by found in Appendix I.3.

5 Related work

Our work belongs to post-hoc concept-based explanations. While training with self-interpretable models (Bouchacourt & Denoyer, 2019; Chen et al., 2019; Lee et al., 2019; Wang & Rudin, 2015) is recommended if the use case allows, often times concepts are not known beforehand which makes the practicality of post-hoc explanations more widely adoptable. Other classes of post-hoc explanations include featured-based explanations (Zintgraf et al., 2017; Petsiuk et al., 2018;

Table 4: Mortality risk attribution with respect to a subset of myocardial infarction complications and comparison with existing medical literature

Complication	CG	TCAV	Excerpted mortality risk description from medical literature
Relapse of MI	3.47	2.55	Recurrent infarction causes the most deaths following myocardial infarction with left ventricular dysfunction. (Orn et al., 2005)
Chronic heart failure	3.27	-1.26	The mortality rate in a group of patients with class III and IV heart failure is about 40% per year, and half of the deaths are sudden. (Bigger, 1987)
Myocardial rupture	1.62	6.52	Myocardial rupture is a relatively rare and usually fatal complication of myocardial infarction (MI). (Shamshad et al., 2010)
Ventricular fibrillation	0.91	1.90	Patients developing VF in the setting of acute MI are at higher risk of in-hospital mortality. (Bougouin et al., 2014)
Dressler syndrome	0.32	-2.85	The prognosis for patients with DS is typically considered to be quite good. (Leib et al., 2017)
Post-infarction angina	-1.40	-2.85	After adjustment, angina was only weakly associated with cardiovascular death, myocardial infarction, or stroke. (Eisen et al., 2016)

Dabkowski & Gal, 2017; Shrikumar et al., 2017; Sundararajan et al., 2017), counterfactual explanations(Dhurandhar et al., 2018; Hendricks et al., 2018; van der Waa et al., 2018; Goyal et al., 2019b; Joshi et al., 2019; Poyiadzi et al., 2020; Hsieh et al., 2021), and sample-based explanations (Bien & Tibshirani, 2011; Kim et al., 2016; Koh & Liang, 2017; Yeh et al., 2018; Pruthi et al., 2020; Khanna et al., 2018). Our work considers the gradient from prediction to concepts, which is in spirit connected to feature explanations which considers the gradient from prediction to feature inputs (Zeiler & Fergus, 2014; Ancona et al., 2017).

Concept-based explanations aims to provide human-centered explanations which answer the question "does this human understandable concept relates to the model prediction?"(Kim et al., 2018; Zhou et al., 2018). Some follows-up for concept-based explanations include when are concept sufficient to explain a model (Yeh et al., 2019), computing interventions on concepts for post-hoc models (Goyal et al., 2019a) and self-interpretable models (Koh et al., 2020), combining concept with other feature attributions (Schrouff et al., 2021), unsupervised discovery of concepts (Ghorbani et al., 2019; Yeh et al., 2020; Ghandeharioun et al., 2021), and debiasing concepts (Bahadori & Heckerman, 2020). The most similar work to ours is the work of Chen et al. (2020), which is motivated by the issue of CAV that concept does not necessarily lie in the linear subspace of some activation layer. They address this problem in the self-explainable model setting by training a self-interpretable model and limits the concepts to be whitened. On the other hand, our work address the non-linear concept problem of CAV in the post-hoc setting by learning a non-linear concept component and connects to the activation space via chain rule. As a result, our method can be applied to the setting when the user has no control of the training process of the model. Another work that considers nonlinear modeling of concepts is that of (Zaeem & Komeili, 2021). They adopted a causal-based interpretation instead and consider the co-occurrence of predicted concepts and target labels to capture the logical causal relation. Their method, albeit also considering non-linear concept modeling, cannot be directly compared to ours since the interpretation logic is fundamentally different.

6 Conclusion

We revisited the fundamental assumptions of CAV, one of the most popular concept-based, gradient interpretation methods. We tackled the problem from a mathematical standpoint and proposed CG to directly evaluate the gradient of a given target model with respect to concepts. Our insight explains the success of CAV, which is a linear special case of CG. Empirical experiments demonstrated that CG outperforms CAV on real datasets and is useful in interpreting models for critical domain applications. Currently CG depends on the representation of input. Devising an input representation invariant method is an interesting future direction. CG also requires user-specified concepts to function. Integrating automatic novel concepts discovery mechanisms into the method may be useful in applications with insufficient domain knowledge.

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A LIMITATIONS

CG is a gradient-based interpretation methods, which is can only be applied to differentiable white-box models. Gradient-based methods convey how small changes in the input affect the output via gradients. Larger changes in the input requires intervention-based causal analysis to predict how the output is affected. As a modification upon CAV, CG also requires users to specify concepts with sufficient representative data samples or close-form concept functions. Sufficient amount of data is more important for CG to prevent the nonlinear function to overfit. Automatic discovery of novel concepts requires introducing other tools. Finally, CG requires fitting non-linear concept models if the concept is provided in the form of representative data samples. This might be computationally intensive for complex non-linear models (e.g. neural networks). The quality of interpretation highly depends on how accurately the concept is captured by the concept model.

B EXAMPLE FOR DEMONSTRATING DIFFERENT CG CALCULATION METHODS

We use a simple toy example to explain the difference between option 1 and 2. Assume $y = x_0 + x_1$ and two concepts $c_0 = x_0, c_1 = x_0 + 0.1x_1$. Since these relationships are all linear, concept gradient will be invariant to reference points. The results computed by option 1 and 2 are

$$\text{Option 1 (individually apply (4)): } R_{c_0,y} = 1, R_{c_1,y} \approx 1.01$$
$$\text{Option 2 (apply CG jointly by (2)): } R_{c_0,y} = -9, R_{c_1,y} = 10$$

At the first glance, it is weird why the contribution of c_0 is negative to y with option 2. But in fact there exists a unique function $y = -9c_0 + 10c_1$ mapping c to y (when jointly considering two concepts), which leads to negative contribution of c_0. This shows that when considering two concepts together as a joint function, the gradient is trying to capture the effect of one concept with respect to others, which may be non-intuitive to human.

C EXAMPLE FOR SELECTING PSEUDO-INVERSE INSTEAD OF OTHER INVERSE MATRICES

For the calculation of CG, multiple inverse matrices exist when $\nabla g(x)$ is not invertible. We gave a high level example in Section 3.4 of why it makes sense to apply the pseudo-inverse. In this example, we provide a concrete example with numbers to further elaborate.

Suppose the raw input x has two dimensions: x_1 indicates the feature "color" and x_2 indicates the feature "shape". There's only one single concept c corresponds to "color", so $c = g(x) = x_1$. The target model is $y = f(x) = x_1 - x_2$.

Let's consider a particular input $\hat{x} = [1, 0]$ and $\hat{c} = 1$. Clearly a small perturbation to "color" can lead to linear change to output with slope 1, so the concept attribution score should be 1. Now let's follow the derivation of CG in this example to show why we choose the minimum-norm solution. Centered at $\hat{c}$, there can be infinite number of (linear) mappings from c to x, but all of them will follow the form according to Theorem 1:

$$h(c) = h(\hat{c}) + \nabla h(\hat{c})(c - \hat{c})$$
$$\nabla h(\hat{c}) = \nabla g(\hat{x})^{\dagger} + G_{\perp}$$

In our example, h can be written explicitly as follows:

$$\begin{aligned} h(c) &= [1, 0] + ([1, 0] + [0, \alpha])(c - 1) \\ &= [c, \alpha(c - 1)], \quad \forall \alpha \end{aligned}$$

This corresponds to Theorem 1, where $\nabla g(\hat{x})^{+} = [1, 0]$ and $G_{\perp}$ is the set of $[0, \alpha]$ with any α. These functions all set $x_1 = c$ but will set $x_2 = \alpha(c - 1)$ with arbitrary α. Conceptually, this is saying there are infinite number of ways to form the mapping from "color" (c) to input (x): we always change "color" according to c but we can arbitrarily change the other orthogonal feature "shape" (x_2) according to color. Concept Gradient is trying to see how the change of c affect output

y while **keeping all the other orthogonal factors fixed**. Therefore, we want to find the mapping that has minimal perturbation to x when changing c, corresponding to keeping all other orthogonal factors fixed. This is the reason to choose the minimal norm solution in pseudo inverse.

In this example, our method sets $\alpha = 0$ and will lead to $h(c) = [1, 0]$. If α is set to some non-zero values in the pseudo-inverse, it will lead to the following score:

$$\frac{\partial f(h(\hat{c}))}{\partial c} = \langle [1, \alpha], [1, -1] \rangle = 1 - \alpha$$

which will give the wrong attribution score for any $\alpha \neq 0$.

D PROOF

Theorem 2. *Let $h : \mathbb{R}^m \to \mathbb{R}^d$ be a smooth and differentiable function mapping c to x and satisfy $g(h(c)) = c$ locally within an ϵ-ball around c_0. Then the gradient of h will take the form of*

$$\nabla h(c_0) = \nabla g(x_0)^{\dagger} + g_{\perp}, \tag{8}$$

where $g_{\perp}$ is in the null space of $\nabla g(x_0)^T$.

Proof. Assume $h : \mathbb{R}^m \to \mathbb{R}^d$ is a function mapping c to x. By Taylor expansion we have

$$g(x') = g(x) + \nabla g(x)^T (x' - x) + O(\|x' - x\|^2) \tag{9}$$

$$h(c') = h(c) + \nabla h(c)^T (c' - c) + O(\|c' - c\|^2), \tag{10}$$

where $x' = h(c')$ and $x = h(c)$. Therefore

$$\begin{aligned} g(x') &= g(x) + \nabla g(x)^T (h(c') - h(c)) + O(\|h(c') - h(c)\|^2) \\ &= g(x) + \nabla g(x)^T \nabla h(c)^T (c' - c) + O(\|\nabla g(x)\|^2 \|c' - c\|^2) + O(\|h(c') - h(c)\|^2). \end{aligned}$$

The last two terms are both $O(\|c - c'\|^2)$ since $\nabla g(x)$ is a constant and h is smooth (thus locally Lipschitz), so

$$c' - c = \nabla g(x)^T \nabla h(c)^T (c' - c) + O(\|c - c\|^2). \tag{11}$$

Therefore, $\nabla g(x)^T \nabla h(c)^T = I$, which means $\nabla h(c) = \nabla g(x)^{\dagger} + g_{\perp}$. □

D.1 DEFINITION OF CONCEPT GRADIENT

Given input space $\mathcal{X}$ and two differentiable functions $f : \mathcal{X} \to \mathcal{Y}$ and $g : \mathcal{X} \to \mathcal{C}$, where $\mathcal{Y}$ is the target label space and $\mathcal{C}$ is the concept label space. We define the concept gradient of $x \in \mathcal{X}$ to attribute the prediction of the model to the concepts:

$$\text{CG}(x) := \nabla f(x) \cdot \nabla g(x)^{\dagger}, \tag{12}$$

where $\nabla g(x)^{\dagger}$ denotes the pseudo-inverse of $\nabla g(x)$. Let $y = f(x) \in \mathcal{Y}$ and $c = g(x) \in \mathcal{C}$. Essentially concept gradient approximates gradient-based saliency of y to c, $h'(c)$, via chain rule. For the case where $\mathcal{X}$, $\mathcal{Y}$, and $\mathcal{C}$ are all scalar fields, the concept gradient exactly recovers $h'(c)$ if $g'(x) \neq 0$ for all $x \in \mathcal{X}$,

Given input space $\mathcal{X}$ and two differentiable functions $f : \mathcal{X} \to \mathcal{Y}$ and $g : \mathcal{X} \to \mathcal{C}$, where $\mathcal{Y}$ is the target label space and $\mathcal{C}$ is the concept label space. Suppose there exist an unknown differentiable function $h : \mathcal{C} \to \mathcal{Y}$ s.t. $f = h \circ g$. Let f', g', and h' denote the first-order derivatives. We define the concept gradient of $x \in \mathcal{X}$ as

$$\text{CG}(x) := \nabla f(x) \cdot \nabla g(x)^{\dagger}$$

where $\nabla g(x)^{\dagger}$ denotes the pseudo-inverse of $\nabla g(x)$. Let $y = f(x) \in \mathcal{Y}$ and $c = g(x) \in \mathcal{C}$. Essentially concept gradient approximates gradient-based saliency of y to c, $h'(c)$, via chain rule. For the case where $\mathcal{X}$, $\mathcal{Y}$, and $\mathcal{C}$ are all scalar fields, the concept gradient exactly recovers $h'(c)$ if $g'(x) \neq 0$ for all $x \in \mathcal{X}$,

$$h'(c) = \frac{\mathrm{d}y}{\mathrm{d}c} = \frac{\mathrm{d}y}{\mathrm{d}x} \cdot \frac{\mathrm{d}x}{\mathrm{d}c} = \frac{\mathrm{d}y}{\mathrm{d}x} \cdot (\frac{\mathrm{d}c}{\mathrm{d}x})^{-1} = f'(x) \cdot \frac{1}{g'(x)} = \text{CG}(x)$$

We now generalize $\mathcal{X}$ to a n-dimensional vector space. Since f, g, and h are differentiable, we can perform Taylor expansion around x and c

$$f(x') = f(x) + \nabla f(x)(x' - x) + O((x' - x)^2) \tag{13}$$
$$g(x') = g(x) + \nabla g(x)(x' - x) + O((x' - x)^2) \tag{14}$$
$$h(c') = h(c) + h'(c)(c' - c) + O((c' - c)^2) \tag{15}$$

Let us denote $\Delta x = x' - x$. We can plug Eq 14 into Eq 15

$$\begin{aligned} h(g(x')) - h(c) &= h'(c)(g(x') - c) + O((g(x') - c)^2) \\ &= h'(c) \cdot \Big(g(x) + \nabla g(x)\Delta x + O(\Delta x^2) - c \Big) + O((g(x') - c)^2) \\ &= h'(c) \cdot \Big(\nabla g(x)\Delta x + O(\Delta x^2) \Big) + O((g(x') - c)^2) \\ &\approx h'(c) \cdot \Big(\nabla g(x)\Delta x \Big) \end{aligned}$$

$$\begin{aligned} f(x') - f(x) &= \nabla f(x)\Delta x + O(\Delta x^2) \\ &\approx \nabla f(x)\Delta x \end{aligned}$$

$$\begin{aligned} h(g(x')) - h(c) &= f(x') - f(x) \\ h'(c) \cdot \Big(\nabla g(x)\Delta x \Big) &\approx \nabla f(x)\Delta x \end{aligned}$$

Let us denote the set of right inverses for $\nabla g(x)$ as $G_r^{-1}(x)$.

$$G_r^{-1}(x) = \{\nabla g(x)^\dagger + g_\perp^T, \forall g_\perp : \langle \nabla g(x), g_\perp \rangle = 0\}$$

By definition for all $g_r^{-1} \in G_r^{-1}(x)$,

$$h'(c) \cdot \Delta x \approx \nabla f(x) \cdot g_r^{-1} \cdot \Delta x$$

If $\nabla g(x)$ is invertible, $G_r^{-1}(x) = \{\nabla g(x)^\dagger\}$ and the equality exactly holds

$$h'(c) = \nabla f(x) \cdot \nabla g(x)^\dagger = \nabla f(x) \cdot \nabla g(x)^{-1}$$

If $\nabla g(x)$ is not invertible, g_r^{-1} is not unique and infinitely many right inverses exist for $\nabla g(x)$. In this case, how does the selection of right inverse relate to interpretation? For interpretation, the goal is to attribute a small change Δc via g_r^{-1} to a small change Δx. Non-invertibility of $\nabla g(x)$ implies there are many ways we could perform the attribution. Consider the alignment between some $g_r^{-1} = \nabla g(x)^\dagger + g_\perp^T$ and $\nabla g(x)$,

$$\frac{\nabla g(x)^{\cdot}(\nabla g(x)^\dagger + g_\perp^T)}{\|\nabla g(x)\| \cdot \|\nabla g(x)^\dagger + g_\perp^T\|} = \frac{\nabla g(x)^{\cdot}\nabla g(x)^\dagger}{\|\nabla g(x)\| \cdot \|\nabla g(x)^\dagger + g_\perp^T\|} \leq \frac{\nabla g(x)^{\cdot}\nabla g(x)^\dagger}{\|\nabla g(x)\| \cdot \|\nabla g(x)^\dagger\|}$$

We argue that the best interpretation is when the attribution is faithful to the relation g between $\mathcal{X}$ and $\mathcal{C}$, i.e., when g_r^{-1} is best aligned with $\nabla g(x)$. Observe that $\nabla g(x)^\dagger$ is in the same direction as $\nabla g(x)$. On the other hand, any right inverse with $g_\perp \neq 0$ is attributing *some* proportion of dc to dx in a direction that is orthogonal to $\nabla g(x)$. Thus, the best choice for g_r^{-1} is $\nabla g(x)^\dagger$.

D.2 CONNECTION WITH CAV

CAV is a special case of concept gradient with g restricted to linear functions. Let $\boldsymbol{v}_c$ denote the concept activation vector associated with concept c. CAV defines the conceptual sensitivity S as the inner product of the input gradient and concept activation vector,

$$S(x) := \nabla f(x) \cdot \frac{\boldsymbol{v}_c}{\|\boldsymbol{v}_c\|}$$

If g is restricted to linear functions,

$$g(x) = \boldsymbol{v}_c^T \cdot x + b_c$$

for some constant bias b_c. Concept gradient is equivalent to CAV conceptual sensitivity normalized by the norm of the concept activation vector,

$$\text{CG}(x) = \nabla f(x) \cdot \nabla g(x)^\dagger = \nabla f(x) \cdot (\boldsymbol{v}_c^T)^\dagger = \nabla f(x) \cdot \frac{\boldsymbol{v}_c}{\|\boldsymbol{v}_c\|^2} = \frac{S(x)}{\|\boldsymbol{v}_c\|}$$

Thus, if the concept can be accurately modeled by a linear function, CAV is capable of retrieving the concept gradient. However, in general the linear separability assumption does not hold. In contrast, concept gradient considers general function classes for g, which better captures the relation between $\mathcal{X}$ and $\mathcal{C}$. Given accurately modeling the concept with g is a necessary condition for correct interpretation, concept gradient is superior to CAV.

E ALTERNATIVE PERSPECTIVE FOR LAYER SELECTION

We can also view layer selection in a typical bias-variance tradeoff perspective. If we selected a later layer to evaluate CG, we are biased towards using a representation of x that is optimized for predicting the target y, not c. However, since the information consists in the representation is less, we also enjoy the benefit of less variance. On the other hand, if we selected an earlier layer to evaluate CG, then we suffer less from the bias (towards y) but is penalized with higher variance due to abundance of information. The optimal layer is where the representation of x is capable of predicting the concept (minimized bias) while no redundant information is available (minimized variance).

We verified the bias-variance tradeoff hypothesis with experiments. More bias (with respect to target labels) in later layers is confirmed with the observation that finetuning more layers yields higher concept prediction accuracy (see Fig 3). Less variance in later layers is confirmed with the experiment below. We repeated the CUB experiments on the Inception v3 model with 5 different random seeds and evaluated the variance of the gradient $\nabla g(x)$ over repeated trials, averaged over all data points. Specifically, the gradients for models finetuned starting from different layers are evaluated on the same layer (`Mixed_6d`) for fair comparison. The results are shown in Fig 4 and confirmed the variance hypothesis.

F ABLATION STUDY ON CONCEPT MODEL CONFIGURATION

Experiments in Section 4.1 and 4.2 shares the same model architecture for the target and concept model. The two design choices here are 1) using the same model architecture and 2) warm-starting the training of concept models with target model weights. The choices are rather straightforward since both models need to share the same input feature representation for the gradients with respect to the input layer to be meaningful. Nevertheless, we conducted an ablation study on the CUB experiment to verify how using different model architectures different weight initialization for the concept model affects interpretation. In this case, CG needs to be evaluated in the input layer, the only layer where the feature representation is shared between target and concept models.

The model architecture alabltion study results are presented in Table 5. The CG scores are all evaluated in the input layer. Evidently, using the same model architecture for both the target and concept models is crucial for good interpretation quality with CG. The degradation of interpretation when using different architectures may be caused by mismatched usage of input feature representation between models. The concept model weight initialization results are presented in Table 6. Using target

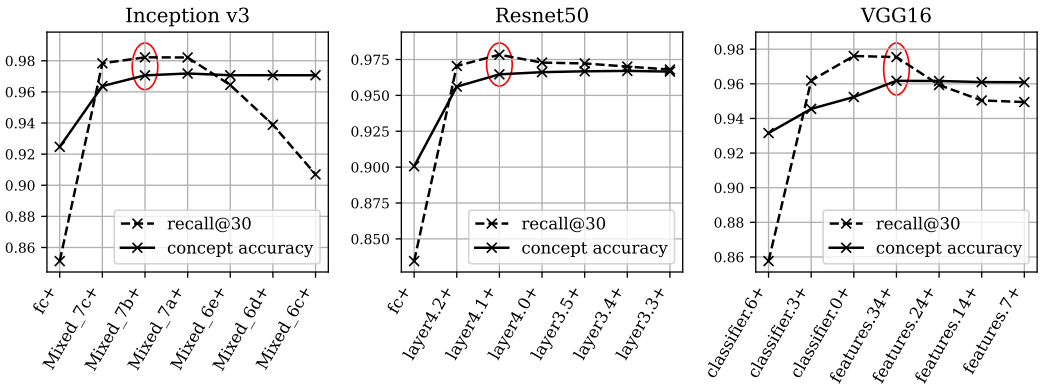

Figure 3: Concept prediction accuracy and concept attribution recall when finetuning starting from different layers of the model. Finetuning more layers leads to higher concept prediction accuracy.

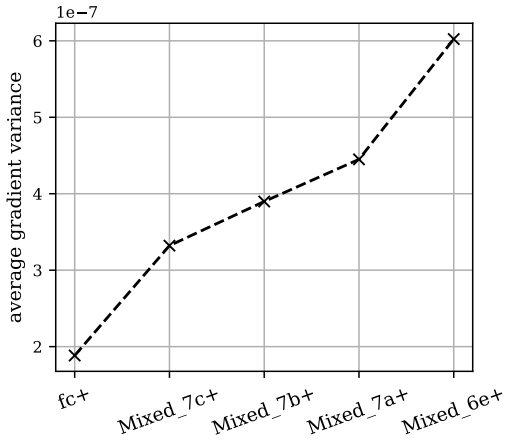

Figure 4: Variance of gradients finetuning starting from different layers. The variance is higher when finetuning starting from earlier layers.

model weights as initialization outperforms using ImageNet pretrained weights significantly. The more similar the pretrained task is to the downstream task is, the better the finetuned performance. In this case, the concept prediction accuracy suggests the target model task of bird classification is a better pretraining task for predicting bird concepts, allowing the concepts to be better captured by the concept function (higher accuracy). This naturally leads to better interpretation results.

Table 5: Ablation study on concept model architecture

Target model	Concept model	R@30	R@40	R@50.
Inception v3	Inception v3	0.872	0.931	0.957
Inception v3	Resnet50	0.535	0.620	0.684
Inception v3	VGG16	0.486	0.561	0.619
Resnet50	Resnet50	0.933	0.976	0.988
Resnet50	Inception v3	0.623	0.705	0.757
Resnet50	VGG16	0.554	0.631	0.692
VGG16	VGG16	0.955	0.986	0.994
VGG16	Inception v3	0.525	0.606	0.664
VGG16	Resnet50	0.609	0.698	0.758

Table 6: Ablation study on concept model weight initialization

Weight initialization	Concept accuracy	R@30	R@40	R@50.
ImageNet pretrained	0.916	0.577	0.670	0.739
target model pretrained	0.972	0.872	0.931	0.957

Table 7: Comparing concept models of different expressiveness. Increasing model expressiveness does not lead to increase in accuracy and thus does not translate to better attribution performance.

Residual Block	Number of Duplication	Concept Accuracy	Local (per-sample)			Global (per-class)		
			R@30	R@40	R@50	R@30	R@40	R@50
layer4.1	1	0.794	0.614	0.718	0.786	0.808	0.909	0.948
	2	0.795	0.605	0.705	0.775	0.810	0.901	0.944
	3	0.791	0.597	0.697	0.767	0.811	0.904	0.944
	4	0.791	0.594	0.693	0.762	0.820	0.906	0.943
layer4.2	1	0.793	0.627	0.726	0.794	0.827	0.915	0.951
	2	0.793	0.622	0.720	0.788	0.838	0.919	0.955
	3	0.794	0.613	0.710	0.777	0.838	0.918	0.952
	4	0.793	0.613	0.712	0.781	0.857	0.931	0.964

G ABLATION STUDY ON THE EXPRESSIVENESS OF CONCEPT MODEL CLASS

In most of this study, the concept model is implemented by finetuning the target model to predict the concepts instead. When using an input representation in deeper layers, the portion of finetuned model would be relatively less, yielding a simpler concept model. Our hypothesis is input representation in deeper layers generally contains higher level semantics and thus only requires simpler models to capture the concept.

To test this hypothesis, we explored whether using a more expressive function class for the concept model benefits the attribution result. We focused on the ResNet architecture and constructed concept models of different complexities. We experimented on input representations in deeper layers (`layer4.1` and `layer4.2`) where the original concept model is simpler and may not be expressiveness enough to capture the concepts. To increase the complexity of a ResNet model, we duplicated ResNet residual blocks. The more times a block is duplicated, the deeper and more expressive a model is.

Table 7 shows the results. The number of duplication represents how many time the selected residual blocks is duplicated for the concept model. As increasing the complexity of the model does not lead to better concept prediction accuracy, the attribution performance (recall) is not improved. This confirmed our hypothesis for using a simpler (more complex) models for deeper (shallower) layer representations.

H TO SMOOTH OR NOT TO SMOOTH?

It has been shown that relying on gradient saliency maps may yield misleading interpretation due to the high non-linearity in deep neural networks. There are many works on improving gradient-based interpretations with respect to the input features (Smilkov et al., 2017; Sundararajan et al., 2017; Shrikumar et al., 2017). Since CG also relies on input gradients for calculation, it is important to examine whether CG suffers from the same issues. In this ablation study, we compared SmoothCG, a variant of CG, that remedies inaccurate gradients.

Inspired by SmoothGrad (Smilkov et al., 2017), we proposed SmoothCG, where the attribution is averaged over the neighborhood D near a data sample.

$$\text{SmoothCG}(x) := \mathop{\mathbb{E}}_{\epsilon \sim D} \text{CG}(x + \epsilon)$$

Smoothing over the neighborhood mitigates inaccurate interpretation caused by abrupt changes in input gradients in highly non-linear functions. It is also shown that randomized smoothing improves the robustness (Cohen et al., 2019). In practice, we take finite samples near an input instance with a predetermined perturbation distribution (e.g. Gaussian) and average their CG scores.

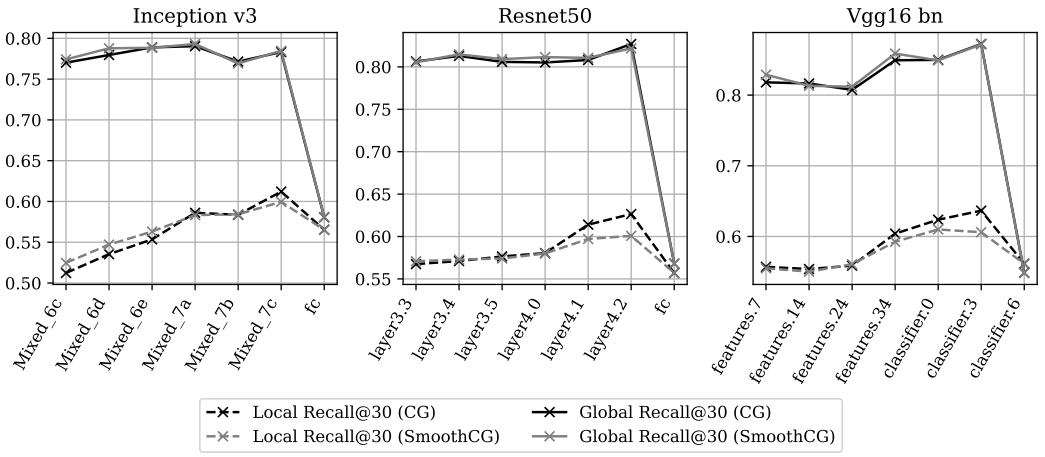

Figure 5: Comparing CUB concept recalls between CG and SmoothCG (stdev=0.01, n=8) for different input representations in various layers and architectures (left to right, deep to shallow layers). SmoothCG performs similarly to CG with marginal improvement in shallow layers.

Figure 5 shows the concept recall comparison between CG and SmoothCG. SmoothCG is calculated by smoothing over 8 samples per instance, adding perturbations sampled from $\mathcal{N}(0, 0.01)$. In general the performances are similar. CG performs marginally better in deeper layers while SmoothCG in shallower ones, likely because gradients propagating to deeper layers are less accurate and thus benefit from the smoothing. However, the difference in performance is not consistent nor significant enough to justify the addition computation cost of SmoothCG.

I Experiment details

I.1 Animal with Attributes 2 (AwA2)

Data preprocessing Since the original task is proposed for zero-shot classification, the class labels in the default training and validation set is disjoint. To construct a typical classification task, we combined all data together then performed a 80:20 split for the new training and validation set. During training, the input images are augmented by random color jittering, horizontal flipping, and resizing, then cropped to the default input resolution of the model architecture (299 for Inception v3, 224 for others). During evaluation, the input images are resized and center cropped to the input resolution.

The attribute labels provided in the dataset contains both concrete and abstract concepts. Some abstract concepts cannot be identified merely by looking at the input image (e.g. new world vs old world). We filtered out 25 attributes that are not identifiable via the input image and used the remaining 60 attributes for interpretation.

Training We trained the target model f with Inception v3 architecture with ImageNet pretrained weights (excluding the final fully connected layer). We optimized with Adam (learning rate of 0.001, beta1 of 0.9, and beta2 of 0.999) with weight decay 0.0004 and schedule the learning rate decay by 0.1 every 15 epochs until the learning rate reaches 0.00001. We trained the model for a maximum of 200 epochs and early stopped if the validation accuracy had not improved for 50 consecutive epochs. The validation accuracy of the trained target model is 0.947.

We trained the concept model g by finetuning different parts of f (freezing different layer model weights). We reweighted the loss for positive and negative class to balance class proportions. We optimized with Adam (learning rate of 0.01, beta1 of 0.9, and beta2 of 0.999) with weight decay 0.00004 and schedule the learning rate decay by 0.1 every 25 epochs until the learning rate reaches 0.00001. We trained the model for a maximum of 200 epochs and early stopped if the validation accuracy had not improved for 50 consecutive epochs.

Evaluation Visualization is conducted on the validation set. Finetuning from `Mixed_7a` is the latest layer that still predicted the concepts well. According to the layer selection guideline, we

selected `Mixed_7a` to evaluate CG. We computed CG with the individual inverse method (4). Fig 6 shows random samples from the validation set and their top 10 rated concepts. These samples are intentionally randomly sampled as opposed to intentionally curated to provide an intuition of the true effectiveness of CG. In general, the retrieved highest ranked concepts are relevant with the input image. In terms of sanity check, there are no contradictions in the concepts (e.g. furry is never assigned to an whales).

Figure 6: Visualization of randomly sampled instances (AwA2 validation set) and the most important concepts associated with their respective CG attribution (top 10 concept, 60 in total).

I.2 CALTECH-UCSD BIRDS-200-2011 (CUB)

Data preprocessing Similar to the AWA2 experiments, the input images are augmented by random color jittering, horizontal flipping, and resizing, then cropped to the default input resolution of the model architecture (299 for Inception v3, 224 for others) during training. During evaluation, the input images are resized and center cropped to the input resolution. We followed (Koh et al., 2020) procedure of removing attributes with insufficient data samples. A total of 112 attributes remains for conducting interpretation. The class attribute labels are assigned as instance labels, i.e., instances from the same class share the same attribute labels.

Training We trained the target model f with three different CNN architectures: Inception v3, Resnet50, and VGG16 (with batch normalization), each with ImageNet pretrained weights (excluding the final fully connected layer). We searched for hyperparameters over a range of learning rates $(0.01, 0.001)$, learning rate schedules (decaying by 0.1 for every $15, 20, 25$ epochs until reaching 0.0001), and weight decay $(0.0004, 0.00004)$. We optimized with the SGD optimizer. We trained the model for a maximum of 200 epochs and early stopped if the validation accuracy had not improved for 50 consecutive epochs. The validation accuracy of the trained target model is 0.797, 0.764, and 0.782 for the three models, respectively.

We trained the concept model g by finetuning different parts of f (freezing different layer model weights). The different layers we started to finetuned from for each model architecture is listed in Table 8. The plus sign in the table represents all layers after the specified layer are all finetuned while all layers prior to the specified layer have their weights kept frozen. We reweighted the loss

Table 8: Finetune layers for architectures

Architecture	Finetuned layers
Inception v3	`fc+`, `Mixed_7c+`, `Mixed_7b+`, `Mixed_7a+`, `Mixed_6e+`, `Mixed_6d+`, `Mixed_6c+`
Resnet50	`fc+`, `layer4.2+`, `layer4.1+`, `layer4.0+`, `layer3.5+`, `layer3.4+`, `layer3.3+`
VGG16	`classifier.6+`, `classifier.3+`, `classifier.0+`, `features.34+`, `features.24+`, `features.14+`, `features.7+`

for positive and negative class to balance class proportions. We searched for the hyperparameters and trained the model same as the target model f.

Evaluation Evaluation is conducted on the testing set. CG and CAV are evaluated in the layer prior to finetuning. We evaluated the recalls for $k = 30, 40, 50$ and generally the recall trend is consistent for all ks. These thresholds are chosen since the number of concepts with positive labels for each instance is in the range of 30 to 40.

I.3 Myocardial Infarction Complications

Table 9: Mortality risk attribution with respect to myocardial infarction complications and comparison with existing medical literature

Complication	CG	TCAV	Excerpted mortality risk description from medical literature
Relapse of MI	3.47	2.55	Recurrent infarction causes the most deaths following myocardial infarction with left ventricular dysfunction. (Orn et al., 2005)
Chronic heart failure	3.27	-1.26	The mortality rate in a group of patients with class III and IV heart failure is about 40% per year, and half of the deaths are sudden. (Bigger, 1987)
Atrial fibrillation	2.29	1.11	AF increases the risk of death by 1.5-fold in men and 1.9-fold in women. (Benjamin et al., 1998)
Myocardial rupture	1.62	6.52	Myocardial rupture is a relatively rare and usually fatal complication of myocardial infarction (MI). (Shamshad et al., 2010)
Pulmonary edema	1.51	2.21	Pulmonary oedema in patients with acute MI hospitalized in coronary care units was reported to be associated with a high mortality of 38–57%. (Roguin et al., 2000)
Ventricular fibrillation	0.91	1.90	Patients developing VF in the setting of acute MI are at higher risk of in-hospital mortality. (Bougouin et al., 2014)
Third-degree AV block	0.69	1.71	In patients with CHB complicating STEMI, there was no change in risk-adjusted in-hospital mortality during the study period. (Harikrishnan et al., 2015)
Ventricular tachycardia	0.51	-0.19	Ventricular tachycardia is most commonly associated with ischemic heart disease or other forms of structural heart disease that are associated with a risk of sudden death. (Koplan & Stevenson, 2009)
Dressler syndrome	0.32	-2.85	The prognosis for patients with DS is typically considered to be quite good. (Leib et al., 2017)
Supraventricular tachycardia	0.24	-0.36	Although SVT is usually not life-threatening, many patients suffer recurrent symptoms that have a major impact on their quality of life. (Medi et al., 2009)
Post-infarction angina	-1.40	-2.85	After adjustment, angina was only weakly associated with cardiovascular death, myocardial infarction, or stroke, but significantly associated with heart failure, cardiovascular hospitalization, and coronary revascularization. (Eisen et al., 2016)