Learning Encoding-Decoding Direction Pairs to Unveil Concepts of Influence in Deep Vision Networks

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Abstract

Empirical evidence shows that deep vision networks represent concepts as directions in latent space, vectors which we call concept embeddings. For each concept, a latent factor—a scalar—indicates the degree of its presence in an input patch. For a given patch, the latent factors of multiple concepts are encoded into a compact vector representation by linearly combining concept embeddings, with the latent factors serving as coefficients. Since these embeddings enable such encoding, we refer to them as encoding directions. A latent factor can be recovered from the representation by taking the inner product with a filter, a vector which we call a decoding direction. These encoding-decoding direction pairs are not directly accessible, but recovering them unlocks significant potential to open the black-box nature of deep networks, enabling understanding, debugging, and improving deep learning models. Decoding directions help attribute meaning to latent codes, while encoding directions help assess the influence of the concept on the predictions, and both directions may assist model correction by unlearning concepts irrelevant to the network's prediction task. Compared to previous matrix decomposition, autoencoder, and dictionary learning approaches which rely on the reconstruction of feature activations, we propose a different perspective to learn these direction pairs. We base identifying the decoding directions on directional clustering of feature activations and introduce signal vectors to estimate encoding directions under a probabilistic perspective. Unlike most other works, we also take advantage of the knowledge encoded in the weights of the network to guide our direction search. For this, we illustrate that a novel technique called *Uncertainty Region Alignment* can exploit this knowledge to effectively reveal interpretable directions that influence the network's predictions. We perform a thorough and multifaceted comparative analysis to offer insights on the fidelity of direction pairs, the advantages of the method compared to other unsupervised direction learning approaches, and how the learned directions compare in relation to those learned with supervision. We find that: a) In controlled settings with synthetic data, our approach is effective in recovering the ground-truth encoding-decoding direction pairs; b) In real-world settings, the decoding directions correspond to monosemantic interpretable concepts, often scoring substantially better in interpretability metrics than other unsupervised baselines; c) In the same settings, signal vectors are faithful estimators of the concept encoding directions validated with a novel approach based on activation maximization. At the application level, we provide examples that demonstrate how the learned directions can help to a) understand global model behavior; b) explain individual sample predictions in terms of local, spatially-aware, concept contributions; and c) intervene on the network's prediction strategy to provide either counterfactual explanations or correct erroneous model behavior.

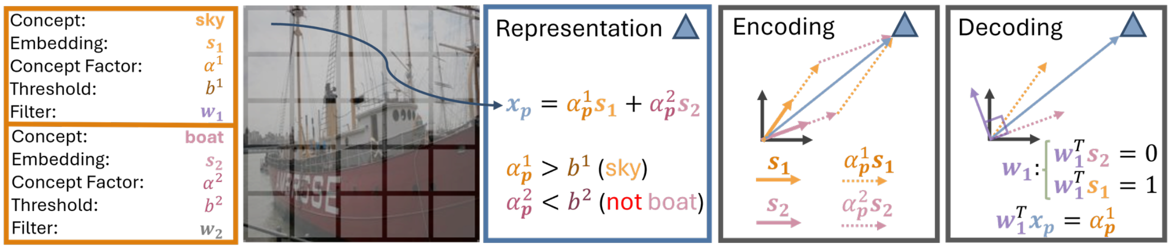

Figure 1: Linear Representation Hypothesis: A hypothesis suggesting that deep networks encode high-level concepts, such as *sky* or *boat*, in distinct directions of their latent space, respectively $\boldsymbol{s}_1$ and $\boldsymbol{s}_2$. The illustration shows the encoding of two concept latent factors (i.e., the degree of concept presence) α^1, α^2 within a patch's representation $\boldsymbol{x_p}$ by utilizing the concept *embedding* directions $\boldsymbol{s}$. Additionally, it demonstrates how a *filter* $\boldsymbol{w}_1$ can be employed to extract one of these latent factors from the representation. The illustration omits depicting the latent space bias for brevity. We use the terms {*encoding* direction, concept *embedding*, *signal* direction} and the terms {*filter*, *decoding* direction} interchangeably throughout this article.

1 Introduction

The linear representation hypothesis suggests that deep neural networks encode high-level concepts in directions of their latent space (Bereska & Gavves, 2024). This hypothesis is sufficiently supported by empirical evidence, mostly by the effectiveness of linear probing. In the latter, a single linear layer can be trained on top of feature representations originating from the upper part of deep neural networks to solve semantic tasks with great success (Szegedy et al., 2014; Alain & Bengio, 2018; Zhou et al., 2018; Kim et al., 2018; Elhage et al., 2022; Nanda et al., 2023). In the concept encoding mechanism suggested by the linear representation hypothesis, the concept content of an input patch is written to its embedding as a linear combination of *concept embeddings*: directions in the latent space represented as vectors, each one associated with a concept. The corresponding scalar coefficient in the linear combination constitutes the concept's latent factor that encodes the degree of concept presence in the input. Due to its utility in encoding the latent factor to a vector representation, we also refer to the concept embedding as the concept's *encoding* or *signal* direction. Retrieving the latent factor back can be accomplished by taking the inner product between the patch embedding and a *filter*, another vector which we term a *decoding* direction. (Fig. 1) An encoding-decoding direction pair is *interpretable* whenever it is related to a concept that is aligned with human intuition; and is *influential* whenever it is related to a concept that the network consistently uses to make predictions. The latter can be quantified using methods for concept sensitivity testing, such as Kim et al. (2018) and Pfau et al. (2020).

On the one hand, since the decoding direction extracts the concept's latent factor from the representation and the concept factor is related to the presence of the concept, it enables understanding of representations, attributing meaning to latent codes (Zhou et al., 2018; Kim et al., 2018). On the other hand, the encoding direction allows one to assess the influence of the concept on the network's predictions (Fel et al., 2023c; Pahde et al., 2024), and both directions may be used to force the network to unlearn concepts irrelevant to its prediction task (Anders et al., 2022; Pahde et al., 2023; Dreyer et al., 2024a). Most previous approaches (Zhou et al., 2018; Kim et al., 2018; Zhang et al., 2021; Fel et al., 2023c; Doumanoglou et al., 2023; Pahde et al., 2024; Doumanoglou et al., 2024) usually focus on identifying decoding or encoding directions in isolation, limiting their applicability to specific appropriate tasks. Moreover, many of them do not explicitly make this distinction and consider using the concepts' decoding directions in use cases where the encoding direction is a better fit. This has recently been pinpointed in the context of concept sensitivity testing and model correction in Pahde et al. (2024).

The encoding - decoding mechanism of concepts for a pre-trained network is not directly accessible. Instead, it is a latent mechanism that needs to be inferred by any means of reverse engineering. Top-down approaches (Zhou et al., 2018; Kim et al., 2018; Pahde et al., 2024) typically guess a concept of interest and subsequently verify whether the network encodes it by linear probing. However, this approach suffers from the need for concept speculation and the access to supervision via expensive annotations. In contrast, bottom-up, unsupervised approaches overcome these limitations, but face significant challenges. Previous unsupervised approaches that attempt to uncover such mechanisms include matrix decomposition (based on principal component analysis or non-negative matrix factorization)(Zhang et al., 2021; Graziani et al., 2023b), sparse autoencoders (SAEs) and dictionary learning (Bricken et al., 2023; Lim et al., 2024; Cunningham et al., 2024; Bussmann et al., 2025). These approaches rely on a decompose-then-reconstruct regime of feature activations. However, attempting to explain every tiny bit of information in the components of latent feature representations is particularly challenging. In addition, not all components may be of interest, as some of them may be noisy distractors (Haufe et al., 2014; Kindermans et al., 2017). Additionally, the reconstruction error of feature activations constitutes dark matter (Engels et al., 2025), which remains largely unexploited. Last, for effective utilization to downstream tasks of interpretability, it is of paramount importance that the identified direction pairs correspond to interpretable concepts, that is, concepts that align as much as possible with human intuition. However, alignment with human intuition should not be a strict criterion, as bottom-up approaches may also reveal counterintuitive concepts that are used by the network to make predictions, possibly exposing an unintended model behavior or a novel strategy to solve a task. SAEs attempt to uncover interpretable direction pairs by learning the directions with a sparsity objective in the units of latent concept factors. However, matrix decomposition approaches do not explicitly optimize for any interpretability criterion.

Unlike previous attempts that rely solely on reconstructing feature activations, in this work we take a different approach in learning the concept encoding-decoding direction pairs. In the proposed approach, we learn the direction pairs jointly, in an unsupervised manner. Decoding directions are identified by **directional clustering** of feature activations and serve as an anchor to estimate encoding directions under a probabilistic perspective. Additionally, we **exploit the network's strategy baked in its weights** when making predictions to guide our direction search. Unlike SAEs that focus on sparsity within units of the latent factors when learning the directions, we emphasize sparsity in the soft binary semantic space of concepts. Our method identifies direction pairs without relying on feature reconstruction, sidestepping the dark matter issue of SAEs Engels et al. (2025) and ignoring noisy distractors in data Haufe et al. (2014); Kindermans et al. (2017), while not being limited by the relative sizes of concept and embedding spaces, which is another limitation when using SAEs. We model the decoding directions using the principles of the recently introduced unsupervised interpretable basis extraction (Doumanoglou et al., 2023) [1], a bottom-up approach that uncovers the directional structure of the embedding space through directional clustering of feature activations. Since concepts are often encoded as directions, this approach has the potential to discover the decoding mechanism of meaningful concepts. This method provides an explicit binary and linear classification rule for concept detection by learning the decoding direction together with an additional threshold to ascertain the presence of a concept. We term this classification rule as a *concept detector* due to its ability to detect the presence of a concept. Additionally, we introduce *signal vectors* that serve as **estimators** for the encoding direction of a concept under a probabilistic perspective, by extending the estimator of a single concept model (Kindermans et al., 2017) to multiple concepts. Furthermore, we also show that the alignment between the uncertainty region of the network, that is, the subspace where the network's predictions are uncertain, with the uncertainty region of the concept detectors, that is, the subspace of ambiguous concept predictions, through a process that we call *Uncertainty Region Alignment* (Fig. 6) can increase the interpretability and influence of the discovered direction pairs.

Our experimental analysis is multifaceted, providing insight into how our method relates to other unsupervised and even supervised direction learning approaches. Using the decoding directions, we assess the ability of our approach to identify interpretable and monosemantic concepts, while we validate the fidelity of signal vectors to the concepts' encoding directions in the challenging real-world settings using a novel approach based on activation maximization (Olah et al., 2017; Nguyen et al., 2019; Fel et al., 2023a). The experiments cover synthetic data with known ground-truth and real-world setups with four families of state-of-the-art deep vision architectures. First, in a controlled setting, the experiments show the efficacy of the proposed approach in identifying the ground-truth concept encoding-decoding direction pairs when previous work fails. Second, in real-world setups, the learned decoding directions identify highly interpretable monosemantic concepts, often scoring significantly higher than the previous unsupervised state-of-the-art baselines in most

[1] Even though it is termed a *basis*, according to our definitions this method identifies decoding directions.

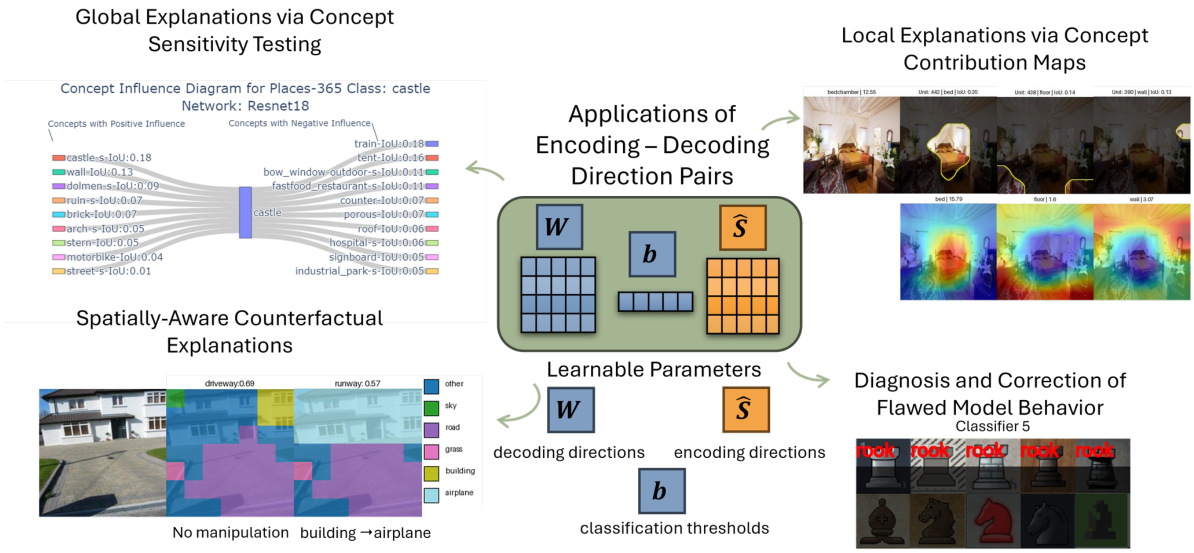

Figure 2: Our Encoding-Decoding Direction Pairs (EDDP) powers a range of applications, highlighting both the generality and the precision of our approach. The figure summarizes applications that we selected to discuss in this work.

of the interpretability metrics, while evidence from the experiment with activation maximization concludes that the encoding-decoding direction pair is faithful, with the learned signal vector being a reliable estimate for the concept's encoding direction. Finally, we demonstrate the utility of our learned directions by i) integrating with the state-of-the-art to address global model behavior understanding, ii) introducing Concept Contribution Maps to provide detailed and spatially-aware local explanations, and iii) providing concrete steps to intervene on the model's prediction strategy, enabling counterfactual explanations and correction of flawed model behavior. Figure 2 summarizes the applications of our method that we selected to discuss in this paper.

2 Related Work

2.1 Direction Learning

We categorize related work into supervised and unsupervised direction learning approaches. In each category, we go through the previous methods, describing the limitations, differences, and similarities with the approach proposed here.

Supervised Concept Direction Learning Typical approaches Zhou et al. (2018); Kim et al. (2018) to concept direction learning make use of a binary linear classifier together with the annotations of a concept dataset. This classifier distinguishes representations of samples with the concept from those without and must rely on the concept content encoded within the representations, thereby requiring its weight vector (filter) to extract (decode) the concept factors from these representations. Known as Concept Activation Vectors (CAVs), these filter weights are approximations to the concept decoding directions, and they are not exact due to possible distractor-noise content in feature components (Haufe et al., 2014; Kindermans et al., 2017; Pahde et al., 2024). Regarding the encoding directions, assuming that the positive cluster contains representations of samples with the concept and the negative cluster contains those without it, Pattern-CAVs (PCAVs (Pahde et al., 2024)) estimate the encoding direction of the concept by computing the difference between the cluster means. These approaches, though, rely on linear probing, requiring the practitioner not only to provide annotations but also to speculate on the name of the concept to be identified. In contrast to that, our approach is unsupervised and bottom-up, reading the structure of the latent space, overcoming both concept speculation and the need for expensive annotations.

Unsupervised Concept Direction Learning A significant amount of related work in unsupervised direction learning is based on methods for matrix decomposition. These methods decompose the matrix of feature activations and may identify the encoding directions of concepts without the need for annotations, but with some limitations. For instance, Principal Component Analysis (PCA) (Graziani et al., 2023a) and Singular Value Decomposition (SVD) (Graziani et al., 2023b) are limited by orthogonality and cannot represent concepts that do not affect variance (Fel et al., 2023b). Likewise, Non-negative Matrix Factorization (NMF) (Zhang et al., 2021; Fel et al., 2023c) only assumes positive components and lacks latent space bias, which limits expressivity. While the transpose of both the PCA matrix and the matrix of the left singular vectors in SVD correspond to the concept decoding directions, NMF lacks a simple equivalent. Instead, at inference time, in which a test sample is examined for its concept content, NMF requires an optimization problem to be solved for each one of the samples, making the approach computationally more expensive than the calculation of an inner product. Our method overcomes all these limitations.

In Dictionary Learning (Bricken et al., 2023; Yun et al., 2023) and Sparse Autoencoders (SAEs) (Sharkey et al., 2022; Cunningham et al., 2024; Bussmann et al., 2025), the goal is to learn decoding-encoding directions by decomposing representations into latent factors and subsequently reconstructing them, and this is done while enforcing sparsity in units of the latent variables. The latter constrains these approaches to be applicable only in cases where the space of latent factors is sufficiently larger than the size of the embedding space. Contrariwise, our method uses a different principle for identifying direction pairs, independent of feature reconstruction, avoiding dealing with the dark matter problem of SAEs (Engels et al., 2025) and the noisy distractor components that may be present in the data (Haufe et al., 2014; Kindermans et al., 2017), while not being restricted by the size of the concept space in relation to the size of the embedding space. This is achieved by enforcing sparsity in the semantic, soft-binary vector space of concepts, instead of sparsity in the units of the latent variables. Since it is independent of feature reconstruction, the proposed approach uses a different way to estimate the concept encoding directions than SAEs, still coupled to the learned decoding directions and the feature activations themselves. Finally, our approach additionally considers linking the directions to their use by the model, a fact that, to our knowledge, is less explored by prior work. More details on the relation of our approach with SAEs can be found in Section A.15.

In contrast to the aforementioned techniques, the method of Doumanoglou et al. (2023; 2024) learns filter directions of linear classifiers, using a concept detector model as in Zhou et al. (2018); Kim et al. (2018), but without requiring supervision. Guided by a sparsity objective and the structure of the latent space, these classifiers map feature representations to a soft-binary concept space, essentially implementing a method for directional clustering. Since the method is guided by the directional structure of the latent space and concepts are often encoded as directions, this process often unveils decoding directions that correspond to highly interpretable, monosemantic concepts. We ground our approach on this model and additionally enhance it by removing orthogonality constraints, feature space standardization, and adding loss terms to a) sustain or improve the interpretability of the identified concepts and b) reduce the impact of distractor-noise on filter weights. Although Doumanoglou et al. (2024) proposed a technique to exploit the utilization of the directions by the network in direction search, our uncertainty region alignment approach shows a notable relative improvement over this previous approach (by up to 22.56% in the interpretability metrics), in 3 of 4 cases. Finally, our work also considers the estimation of concept encoding directions, an aspect that was not addressed in these previous works. More details on this comparison can be found in Section A.2.

2.2 Applications of Directions

Our learned direction pairs enable a series of applications, from global model understanding and detailed spatially-aware local explanations down to model intervention, which allows for counterfactual explanations and model correction. Typical previous enablers of such applications are the Concept Bottleneck Models (CBMs) (Koh et al., 2020). The principal idea behind CBMs is to create an inherently interpretable model which is comprised of a backbone, a concept bottleneck, and a linear head. This model makes class predictions in two steps. In the first, the concept bottleneck predicts the concept content of the image based on the features extracted from the backbone, while in the second, the head predicts the image class based on the previously extracted concept content. What makes this architecture interpretable is the fact that the concept vector, i.e, the output of the concept bottleneck, is trained to have each dimension aligned with an interpretable concept. More recent CBM variants (Yuksekgonul et al., 2023; Oikarinen et al., 2023) proposed techniques to turn any non-interpretable model into a CBM. For the latter, the original model's backbone is kept frozen and the last linear head is discarded. Instead, a concept bottleneck is introduced as a projection layer that translates the embeddings of the backbone to the concept space. Finally, a last sparse linear head maps the concept vector to the output classes. To learn the concept bottleneck without annotations, Yuksekgonul et al. (2023); Oikarinen et al. (2023) leveraged CLIP Radford et al. (2021), whose visual prompt capabilities (Shtedritski et al., 2023) were later exploited by Benou & Raviv (2025) to train a concept bottleneck that is additionally spatially-aware. This last approach can localize concept content within the input image, improving upon previous methods that could only predict concepts at the image level rather than at the patch level. Finally, recently, Rao et al. (2024) leveraged SAEs (Cunningham et al., 2024) to learn a CBM for CLIP itself.

All these approaches require training the last sparse linear head with access to the model's training dataset. Furthermore, some of them also require a dataset with concept annotations or utilize a foundation model (CLIP) to learn the concept bottleneck. Unlike all of them, our work is fundamentally different, enabling all the previous applications while remaining completely non-intrusive without the need to train any network components. Overall, in this work, we show that it is possible, at least to some extent, to get the benefits of CBMs without the need to train additional heads, access concept annotations, or precisely reconstruct features. We discover directions that correspond to concepts that the model already knows and subsequently we harness them in applications of mechanistic interpretability (Saphra & Wiegreffe, 2024; Kästner & Crook, 2024; Bereska & Gavves, 2024).

3 Background

The latent factor of a concept is a scalar linked to the concept's presence, embedded in the latent space via multiplication with its encoding direction, also called the concept's **signal** direction. For this reason, we also refer to this latent factor as the **signal value**. Feature activations are considered as linear combinations of signals and noisy directional components called **distractors**. In the proposed approach, a **filter** is a decoding direction that, through the inner product with a feature representation, extracts the signal's value. Below we provide a more formal explanation of these terms and provide details essential to understand our contributions.

3.1 Preliminaries

Let $\boldsymbol{X} \in \mathbb{R}^{H \times W \times D}$ denote the feature representation of an image in an intermediate layer of a deep neural network with spatial dimensions $H, W \in \mathbb{N}^+$ and latent space dimensionality $D \in \mathbb{N}^+$. Let also $\boldsymbol{x_p} \in \mathbb{R}^D$ denote a **pixel** element of this representation at the spatial location $\boldsymbol{p} = (w, h)$, $w \in \{0, 1, ..., W-1\}, h \in \{0, 1, ..., H-1\}$. Since $\boldsymbol{x_p}$ is related to a patch within the input image of the network, we also refer to it as **patch embedding**.

3.2 Signals, Distractors, Filters, Concept-Detectors

In encoding a single concept i, Kindermans et al. (2017); Pahde et al. (2024) proposed a model for the data generation process of feature representations: $\boldsymbol{x_p} = \alpha_{\boldsymbol{p}} \boldsymbol{s}_i + \beta_{\boldsymbol{p}} \boldsymbol{d}$, $\boldsymbol{s}_i, \boldsymbol{d} \in \mathbb{R}^D, \alpha_{\boldsymbol{p}}, \beta_{\boldsymbol{p}} \in \mathbb{R}$. Here, $\boldsymbol{s_i}$ is the **signal** direction that carries the information of whether $\boldsymbol{x_p}$ is part of concept i. The concept information lies within the **signal value** $\alpha_{\boldsymbol{p}}$. Larger $\alpha_{\boldsymbol{p}}$ suggests greater confidence that $\boldsymbol{x_p}$ belongs to concept i. $\boldsymbol{d}$ is the **distractor** direction, modeling noise, or information not related to the concept. $\beta_{\boldsymbol{p}}$ follows a random distribution, typically the gaussian or uniform distribution, and is **independent** of whether $\boldsymbol{x_p}$ belongs to concept i. According to Kindermans et al. (2017), the value of the signal $\alpha_{\boldsymbol{p}}$ can be extracted using a **regression filter** $\boldsymbol{w}_i$ and the inner product: $z_{\boldsymbol{p},i} = \boldsymbol{w}_i^T \boldsymbol{x_p} = \alpha_{\boldsymbol{p}} \boldsymbol{w}_i^T \boldsymbol{s}_i + \beta_{\boldsymbol{p}} \boldsymbol{w}_i^T \boldsymbol{d}$, if we choose $\boldsymbol{w}_i : \boldsymbol{w}_i \perp \boldsymbol{d}$, and $\boldsymbol{w}_i^T \boldsymbol{s}_i = 1$. Let σ denote the sigmoid function. Since stronger values of $\alpha_{\boldsymbol{p}}$ indicate more confidence in concept presence, when combined with a threshold $b_i \in \mathbb{R}$ that can be learned from data, this regression filter can be turned into a **concept detector**: $y_{\boldsymbol{p},i} = \sigma(z_{\boldsymbol{p},i} - b_i)$, essentially a binary classifier that can answer the question of whether $\boldsymbol{p}$ belongs to concept i.

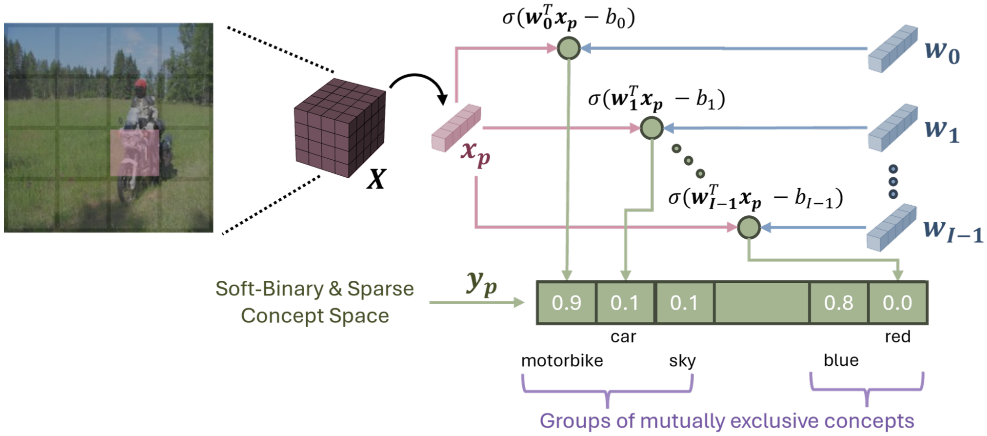

Figure 3: The core concept of Unsupervised Interpretable Basis Extraction (UIBE Doumanoglou et al. (2023)) is to learn a set of concept detectors, which are essentially binary linear classifiers with learnable filters and biases. These detectors aim to transform feature representations to the soft-binary vector space of concepts in which the newly transformed representations are sparse. In this procedure the input to the method is the network features corresponding to images coming from a concept dataset (without the need for annotations) and the only learnable parameters are the previously mentioned filters and biases themselves. Identifying the concept name behind each detector is done in a post-processing step with a procedure we refer to as *Direction Labeling*.

With access to the signal value, Haufe et al. (2014); Kindermans et al. (2017) offer a formula to estimate the concept's signal direction:

$$\hat{\boldsymbol{s}}_i = \frac{\mathrm{cov}[\boldsymbol{x_p}, \alpha_{\boldsymbol{p}}]}{\mathrm{var}[\alpha_{\boldsymbol{p}}]} = \frac{\mathrm{cov}[\boldsymbol{x_p}, z_{\boldsymbol{p},i}]}{\mathrm{var}[z_{\boldsymbol{p},i}]} \tag{1}$$

3.3 Unsupervised Interpretable Direction Learning

Recent research (Doumanoglou et al., 2023) introduced an unsupervised method to identify concepts from the structure of the latent space. Motivated by the directional encoding of concepts, the method partitions the latent space into linear regions, each represented by a hyperplane and a normal vector, forming clusters. Feature activations from an unlabeled *concept dataset*, possibly activations of images from the network's training set, are assigned to these clusters. The method learns $\boldsymbol{W}$ and $\boldsymbol{b}$ of a feature-to-cluster membership function, a mapping to the semantic space, with $\boldsymbol{y_p} = \sigma(\boldsymbol{W}^T\boldsymbol{x_p} - \boldsymbol{b}) \in [0,1]^I, \boldsymbol{W} \in \mathbb{R}^{D\times I}, \boldsymbol{b} \in \mathbb{R}^I$, and I as the cluster count. By softly assigning features to a small number of clusters, the interpretability of the clustering is improved. This is grounded in the idea that an image patch generally holds only a few semantic labels from a larger set, reflecting sparsity in the semantic space. Sparsity in the assignments is achieved using two loss terms: the first is *Sparsity Loss* ($\mathcal{L}^s$), and the second is *Maximum Activation Loss* ($\mathcal{L}^{ma}$), which ensures binary cluster membership:

$$\begin{aligned} &\mathcal{L}^s = \mathbb{E}_{\boldsymbol{p}}\big[\mathcal{L}^s_{\boldsymbol{p}}\big], \quad \mathcal{L}^{ma} = -\mathbb{E}_{\boldsymbol{p}}\big[\boldsymbol{q}_{\boldsymbol{p}}^T \log_2(\boldsymbol{y_p})\big], \\ &\mathcal{L}^s_{\boldsymbol{p}} = \mathcal{H}(\boldsymbol{q_p}), \quad \boldsymbol{q_p} = \frac{\boldsymbol{y_p}}{||\boldsymbol{y_p}||_1} \end{aligned} \tag{2}$$

with $\mathcal{H}$ denoting entropy. Under a different interpretation perspective, a column of $\boldsymbol{W}$ together with a corresponding element of $\boldsymbol{b}$ (i.e., $\boldsymbol{w}_i, b_i$) forms a linear classifier or concept detector $y_{\boldsymbol{p},i} = \sigma(\boldsymbol{w}_i^T\boldsymbol{x_p} - b_i)$. This method also optimizes linear separability by minimizing the inverse of the classification margin $M_i = \frac{1}{||\boldsymbol{w}_i||_2}$ (*Maximum Margin Loss* - $\mathcal{L}^{mm}$) and penalizes clusters with few assignments using the *Inactive Classifier Loss* - $\mathcal{L}^{ic}$ (Doumanoglou et al., 2024) (See Fig. 3 and more details in Section A.1). Despite the potential misalignment with human intuition, the sparse nature of the feature-to-cluster assignments facilitates concept definition or identification.

3.4 Direction Labeling

When learning directions in an unsupervised manner, the name of the concept represented by each encoding-decoding direction pair is unknown. In a real-world setting, the concept name could be identified by manually inspecting the samples that (maximally) activate the decoding direction. However, in a benchmark setting, where interpretability needs to be quantified in terms of metrics and without human involvement, it is necessary to automate the assignment of a concept label to each of the direction pairs. We refer to this process as *direction labeling* and employ Network Dissection Bau et al. (2017) for its implementation. In essence, Network Dissection assigns a semantic label to each of the concept detectors based on their segmentation performance in a dataset with annotated concepts. Although it was originally proposed as a method to assign labels to each of the basis vectors in the natural latent space basis, Network Dissection is capable of assigning labels to any set of directions after basis change. Despite possible biases against unsupervised learning due to annotation limitations, we adopt and expand on this labeling protocol as a best-effort approach to evaluate the interpretability of our concept detectors and the rest of the unsupervised state-of-the-art.

3.5 Concept Sensitivity Testing

Given the intermediate representation of an image belonging to class k and the direction of concept c in the latent space, RCAV (Pfau et al., 2020) measures the sensitivity of the model to concept c when predicting class k. This is accomplished by perturbing the representation towards the direction of the concept with strength α, and subsequently comparing the output probability of the network for the same class before and after the perturbation. Subsequently, an overall dataset score in the range $[-1, 1]$ is computed, where zero means inconsistent use of the concept by the model, while extremes indicate consistent and strong positive or negative concept contributions to predict class k. A statistical test compares concept sensitivity against sensitivity towards random directions to ensure significance. In our evaluations, we refer to *directions of significant influence* in cases where the directions meet the criteria of this statistical significance test. Although the initial work used CAVs to test concept sensitivity, a recent study (Pahde et al., 2024) suggests that the appropriate direction for this purpose is the concept's encoding direction, an aspect that we consider in our evaluations.

4 Method

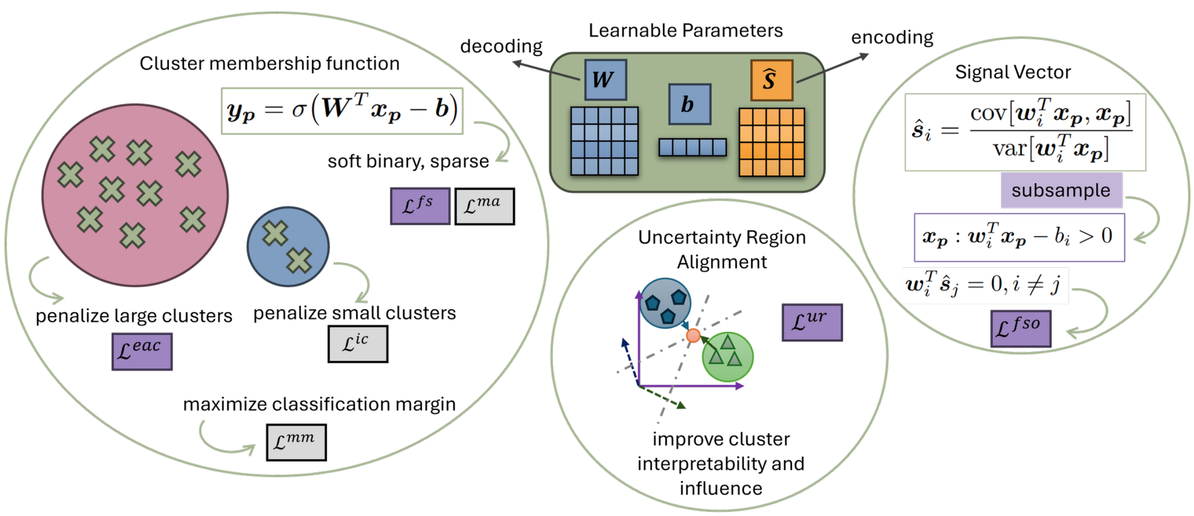

Figure 4: The proposed method analyzes the latent space to uncover its directional structure. Because many concepts are naturally encoded as specific directions, this process often reveals the encoding-decoding mechanism of meaningful, monosemantic, and highly interpretable concepts. The figure depicts an overview of the method's components. $\mathcal{L}$ denotes loss terms. **Purple** indicates contributions of this work, while **light gray** indicates loss terms from Doumanoglou et al. (2023; 2024).

For a specific network layer, our method receives as input the feature representations of images sourced from a *concept dataset*, that is, an unlabeled dataset of images coming from the domain of the network depicting concepts that the network might use to make predictions, and utilizes the upper part of the network f^+ after the layer of study. The aim of our approach is to *read* the structure of the embedding space in the specific layer and learn encoding-decoding direction pairs that explain this structure. Since concepts are often encoded in latent space directions, reading the structure may reveal the mechanisms to encode and decode meaningful, monosemantic, and highly interpretable concepts. The method is unsupervised, and therefore, the identified direction pairs may correspond to concepts that do not align with human intuition. However, they reflect clear directional clusters in the latent space of the network. Thus, this approach has the potential to reveal erroneous strategies exploited by the model to make predictions (Section 7.11). In an attempt to make these clusters as meaningful as possible, we optimize for a sparsity property of interpretability in the feature-to-cluster assignments (Section 3.3). Additionally, to ensure that those clusters are influential to the network's predictions, we exploit the uncertainty region of the model.

We extend the previous signal-distractor data model (Section 3.2) from the encoding of a single concept to multiple concepts (Section 4.1) and learn concept detectors $\{\boldsymbol{W}, \boldsymbol{b}\}$ using the objectives of Section 3.3. In the new data model, we remove the constraints of Doumanoglou et al. (2023) regarding feature space standardization and the orthogonality between filters, allowing for a more flexible clustering which, as we show in the experiments, reduces redundancy. However, when lifting those constraints, we found that they additionally acted as regularizers that prevented direction collapse and trivial clustering; thus, we address their removal with additional loss terms discussed in Section 4.2 that sustain or even improve the interpretability of the clustering. We additionally estimate concept signal directions using learnable **signal vectors** $\hat{\boldsymbol{s}}_i$ (Section 4.3). Furthermore, we propose Uncertainty Region Alignment (Section 4.4), a loss that can assist in improving the interpretability of the directions or in aligning signal vectors with directions of significant influence. Finally, we propose to learn the direction pairs using ϵ-constrained optimization via the Augmented Lagrangian Loss which we describe in Section 4.5. In summary, concept detectors and signal vectors are learned together in an end-to-end process, influenced by the losses of Sections 3.3, 4.2, 4.3, and 4.4 under the optimization scheme of Section 4.5. An overview of our method and the interconnections between its components is provided in Figures 4 and 5.

4.1 Multi-Concept Signal-Distractor Data Model

We introduce an extended signal-distractor data model for the latent space, which models the encoding of **multiple** concepts. Each patch embedding $\boldsymbol{x_p}$ is considered as a linear combination of latent concept signals $\boldsymbol{S} \in \mathbb{R}^{D \times I}$ and distractors $\boldsymbol{D} \in \mathbb{R}^{D \times F}, F \leq D - I$. We also consider a latent space bias $\boldsymbol{c} \in \mathbb{R}^D$, common for all $\boldsymbol{x_p}$.

$$\boldsymbol{x_p} = \boldsymbol{S}\boldsymbol{\alpha_p} + \boldsymbol{D}\boldsymbol{\beta_p} + \boldsymbol{c} \tag{3}$$

with $\boldsymbol{\alpha_p} \in \mathbb{R}^I$ and $\boldsymbol{\beta_p} \in \mathbb{R}^F$. $\boldsymbol{S}$ is a matrix of $I \in \mathbb{N}^+$, D-dimensional, unit-norm concept signal directions and $\boldsymbol{D}$ a matrix denoting a basis for distractor components. Each signal direction encodes the presence of a distinct concept. We apply the same assumptions for individual signal values $\alpha_{\boldsymbol{p},i}$ (the i-th element of $\boldsymbol{\alpha_p}$) and distractor coefficients $\beta_{\boldsymbol{p},f}$ as in Section 3.2. Finally, we further assume that only a limited number of semantic concepts are assigned to $\boldsymbol{x_p}$, among many possible semantic labels.

4.2 Interpretability Losses to Recover Implicit Regularizations

We propose **Self-Weighted Reduction** ($\mathcal{R}_{SW}$) as an aggregation method to estimate the maximum element in a set. Consider the set of elements $\{\zeta_k\}$, $\zeta \in \mathbb{R}^+, k \in \mathbb{N}$. The Self-Weighted Reduction is defined as:

$$\mathcal{R}_{SW}(\{\zeta_k\}) = \frac{\sum_k \zeta_k^{\nu+1}}{\sum_k \zeta_k^{\nu}} \tag{4}$$

which is equal to the weighted average of elements in $\{\zeta_k\}$ with each element being weighted by ζ_k^ν, $\nu \geq 1, \nu \in \mathbb{R}^+$ a sharpening factor. This aggregation may be seen as a soft differentiable version of the max operation, since the largest value in the set $\{\zeta_k\}$ is weighted with the largest weight.

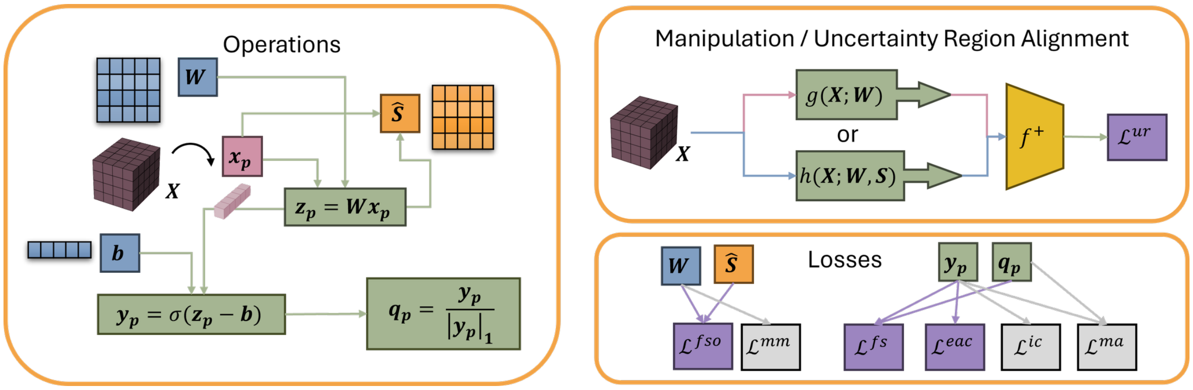

Figure 5: **Left**: The learnable parameters of the method $\hat{\boldsymbol{S}}, \boldsymbol{W}, \boldsymbol{b}$ and intermediate variables $\mathbf{z_p}, \boldsymbol{y_p}, \boldsymbol{q_p}$. **Top Right**: Feature manipulation and Uncertainty Region Alignment. **Bottom Right**: Loss terms $\mathcal{L}$ with their dependencies. **Purple** indicates loss contributions of this work, while **light gray** indicates loss terms from Doumanoglou et al. (2023; 2024).

Excessively Active Classifier Loss ($\mathcal{L}^{eac}$) This loss penalizes excessively large clusters to prevent trivial solutions where all inputs are assigned to a single cluster. It relies on a hyper-parameter $\rho \in (0, 1)$, similar to sparse autoencoders Ng et al. (2011), which sets a proportional bound on cluster size. The unreduced formula for the i-th cluster is below, with $\gamma > 1, \gamma \in \mathbb{R}^+$ as a sharpening factor, $1 - \rho$ normalizing the loss in the range $[0, 1]$ and $\boldsymbol{p}$ varying across all pixels and image representations in the concept dataset:

$$\mathcal{L}_i^{eac} = \frac{1}{1-\rho} \mathrm{ReLU}(\mathbb{E}_{\boldsymbol{p}}[y_{\boldsymbol{p},i}^{\gamma}] - \rho) \tag{5}$$

The final loss uses $\mathcal{R}_{SW}$: $\mathcal{L}^{eac} = \mathcal{R}_{SW}(\{\mathcal{L}_i^{eac}, i \in \{0, 1, ..., I-1\}\})$

Focal Sparsity Loss ($\mathcal{L}^{fs}$) Inspired by Focal Loss (Lin et al. (2017)), we introduce **Focal Sparsity Loss**, which puts more emphasis on sparsifying the feature-to-cluster assignments of the most challenging patch embeddings. To this end, for each $\boldsymbol{x_p}$ we calculate a coefficient $\theta_{\boldsymbol{p}} \in [0, 1]$, which is related to the number of clusters assigned to $\boldsymbol{x_p}$:

$$\theta_{\boldsymbol{p}} = 1 - (\mathcal{R}_{SW}(\{\boldsymbol{q}_{\boldsymbol{p},i}, i \in \{0, 1, ..., I-1\}\}))^{\mu}, \mu \in \mathbb{R}^+ \tag{6}$$

with μ a sharpening factor and $\boldsymbol{q_p} \in [0, 1]$ an intermediate variable with elements inversely proportional to the patch's number of cluster assignments, calculated as in (2). If $\mathcal{L}_{\boldsymbol{p}}^s$ (2) denotes the *Sparsity Loss* for pixel $\boldsymbol{p}$, the *Focal Sparsity Loss* is defined as:

$$\mathcal{L}^{fs} = \frac{\sum_{\boldsymbol{p}} \theta_{\boldsymbol{p}} \mathcal{L}_{\boldsymbol{p}}^s}{\sum_{\boldsymbol{p}} \theta_{\boldsymbol{p}}} \tag{7}$$

Similar to the previous case, in (7) $\boldsymbol{p}$ varies across all spatial elements and image representations in the concept dataset. When we use *Focal Sparsity Loss* we use it as a replacement for the *Sparsity Loss* $\mathcal{L}^s$ of Doumanoglou et al. (2023).

4.3 Signal Vectors as Concept Signal Estimators

In this paragraph, we consider the new data model that was outlined in Section 4.1 and try to validate whether (1) can be used to estimate the signal direction of a concept. Suppose that our objective is to estimate the signal direction of concept i when we have access to a collection of patch embeddings $\{\boldsymbol{x_p}\}$ and their signal values $\{\alpha_{\boldsymbol{p},i}\}$. Starting from the approach of Kindermans et al. (2017), it is easy to prove that whenever $a_{\boldsymbol{p},i}$ is independent of all $a_{\boldsymbol{p},j}, j \neq i$ and $\beta_{\boldsymbol{p},f}$ the following property holds: $\mathrm{cov}[\boldsymbol{x_p} - a_{\boldsymbol{p},i}\boldsymbol{s}_i, a_{\boldsymbol{p},i}] = 0$, which, according to Kindermans et al. (2017) directly implies that (1) can be utilized to estimate the direction of the signal.

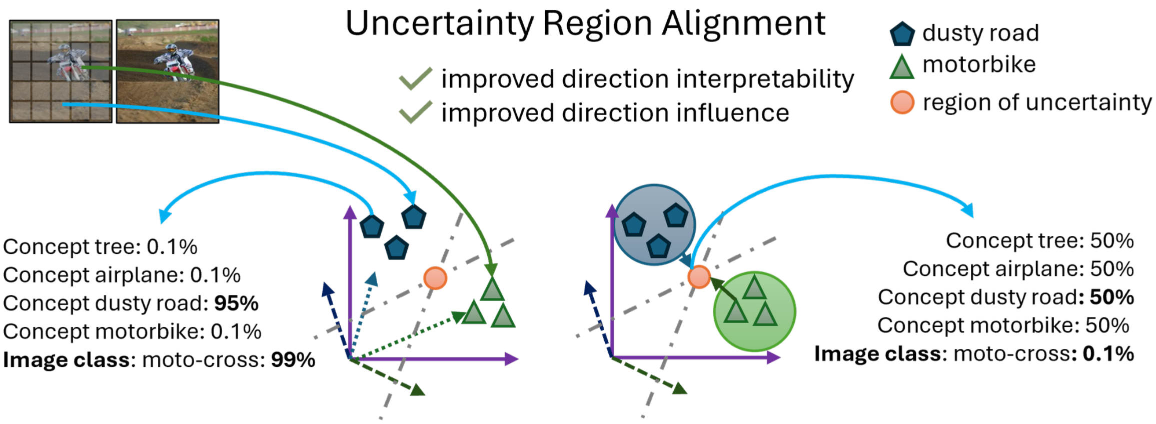

Figure 6: The uncertainty region of the network is defined as the subspace where all network's predictions are maximally uncertain. The uncertainty region of the concept detectors is defined as the intersection of all their decision hyperplanes, i.e. the subspace of ambiguous concept predictions. Aligning these two through feature manipulation may improve direction pair interpretability or serve as a balance between the interpretability and influence of the learned direction pairs.

However, while $a_{\boldsymbol{p},i}$ can be considered independent of distractor coefficients $\beta_{\boldsymbol{p},\boldsymbol{f}}$ that represent noise, the independence assumption between $a_{\boldsymbol{p},i}$ and $a_{\boldsymbol{p},j}, j \neq i$ is easily violated in practice. Some pairs of variables $a_{\boldsymbol{p},i}$ and $a_{\boldsymbol{p},j}, j \neq i$ may indeed be independent and this would be the case when concepts i and j belong to different groups of mutually-exclusive concepts, for example when concept i belongs to the group of *objects* and concept j to the group of *colors* and the concepts of the first group are independent of those of the second. However, when the concepts i and j belong to the same group of mutually exclusive concepts (for instance, when concept i corresponds to *car* and concept j to *tree* and both concepts belong to the group of *objects*), there may be an anti-correlated relationship between the variables $a_{\boldsymbol{p},j}$ and $a_{\boldsymbol{p},i}, j \neq i$ due to the fact that whenever $a_{\boldsymbol{p},i} > b_i$, $a_{\boldsymbol{p},j} < b_j$. However, the latter bias can be eliminated if we consider only samples with the concept instead of both positive and negative samples. In that case, among that subset of the data, the signal values $a_{\boldsymbol{p},i}$ and $a_{\boldsymbol{p},j}$ can be considered independent by assumption, as we now removed the biases b_i, b_j due to sub-sampling. This allows us to still consider (1) as a signal estimator, even under the extended data model of multiple concepts, provided that in the computation of the covariance and variance terms of (1) we subsample the patch embeddings based on their concept label, i.e. keep only samples with the concept, instead of additionally considering samples without it. The latter can be easily accomplished when employing the respective concept detector.

We refer to the signal estimator of concept i that is obtained under these conditions as the **signal vector** $\hat{\boldsymbol{s}}_i$. However, we still require access to the signal values. As explained in Section 3.2, estimating signal values can be attributed to the filters of the concept detectors. They can serve this purpose if the weight vector $\boldsymbol{w}_i$ is orthogonal to all $\boldsymbol{s}_j$ where $j \neq i$, as well as the distractor subspace $\boldsymbol{D}$.

Thus, we employ the following **Filter-Signal Vector Orthogonality Loss** when learning the directions:

$$\mathcal{L}^{fso} = \sqrt{\mathbb{E}_{i,j}\left[((1-\delta_{i,j})\bar{\boldsymbol{w}}_i^T \bar{\boldsymbol{s}}_j)^2\right]} \tag{8}$$

with $\delta_{i,j}$ the kronecker delta and $\bar{\boldsymbol{w}}, \bar{\boldsymbol{s}}$ denoting the L2-normalized filter weights and signal vectors.

To achieve accurate signal value extraction, $\boldsymbol{w}_i$ should additionally be orthogonal to the distractor basis; however, we do not explicitly estimate the distractors. Instead, we use the Uncertainty Region Alignment loss from Section 4.4 to ensure alignment of the directions with utilization by the network.

4.4 Uncertainty Region Alignment to Discover Meaningful Concepts of Influence

The presence or absence of a concept in a representation can provide neutral, supportive, or opposing evidence against the prediction of a class. Since the concept-class pair association is unknown when learning concept directions, a straightforward strategy to perform concept arithmetic on the features in order to find their utility by the network lacks ground-truth information on how concepts affect class predictions. To overcome this difficulty, we can make a simple but more elegant hypothesis that uncertain network predictions occur when the representation has ambiguous concept information. We propose improving the direction search by aligning the uncertainty regions of the network and the concept detectors. The *uncertainty region of the network* is the subspace where its predictions are most uncertain, and the *uncertainty region of the concept detectors* is the subspace where their decision hyperplanes intersect. Figure 6 illustrates the concept of Uncertainty Region Alignment.

To accomplish the alignment, **all** the patch embeddings $\boldsymbol{x_p}$ in an image are manipulated towards the direction $-\boldsymbol{dx_p}$ to arrive at $\boldsymbol{x'_p} = \boldsymbol{x_p} - \boldsymbol{dx_p}$. Based on our estimates of $\boldsymbol{w}_i$, b_i, and $\hat{\boldsymbol{s}}_i$, we select the direction $\boldsymbol{dx_p}$ so that the shifted $\boldsymbol{x'_p}$ lies at the intersection of the concept detectors' decision hyperplanes. Then, we ensure the network's prediction for the resulting manipulated image representation is highly uncertain, effectively aligning both uncertainty regions. More specifically, we define two types of feature manipulation for this purpose:

Unconstrained Feature Manipulation (UFM) in which $\boldsymbol{x'_p} = g_{\boldsymbol{p}}(\boldsymbol{x_p}; \boldsymbol{W}) = \boldsymbol{x_p} - \boldsymbol{dx_p}$ and $\boldsymbol{dx_p}$ such that:

$$\begin{aligned} \boldsymbol{w}_i^T \boldsymbol{x'_p} - b_i = 0 &\Rightarrow \boldsymbol{w}_i^T (\boldsymbol{x_p} - \boldsymbol{dx_p}) - b_i = 0, \forall i, \\ \boldsymbol{W}^T (\boldsymbol{x_p} - \boldsymbol{dx_p}) - \boldsymbol{b} = \boldsymbol{0} &\Rightarrow \boldsymbol{dx_p} = (\boldsymbol{W}^T)^+ (\boldsymbol{W}^T \boldsymbol{x_p} - \boldsymbol{b}) \end{aligned} \tag{9}$$

with $\boldsymbol{A}^+$ denoting the pseudo-inverse of $\boldsymbol{A}$.

Constrained Feature Manipulation (CFM) in which we avoid manipulating features towards datapoints that fall outside the concept encoding manifold of the network, by restricting feature manipulation to occur within the span of the signal vectors, i.e. $\boldsymbol{dx_p} = \hat{\boldsymbol{S}} \boldsymbol{v_p}$, $\boldsymbol{v_p} \in \mathbb{R}^I$, with $\hat{\boldsymbol{S}} \in \mathbb{R}^{D \times I}$ denoting the matrix whose columns correspond to the learned signal vectors $\hat{\boldsymbol{s}}_i, i \in \{0, 1, ..., I-1\}$. The feature manipulation formula for a patch embedding $\boldsymbol{x_p}$ is $h_{\boldsymbol{p}}(\boldsymbol{x_p}; \boldsymbol{W}, \hat{\boldsymbol{S}}) = \boldsymbol{x_p} - \boldsymbol{dx_p}$, with $\boldsymbol{dx_p}$ given by:

$$\begin{aligned} \boldsymbol{w}_i^T \boldsymbol{x'_p} - b_i = 0 &\Rightarrow \boldsymbol{w}_i^T (\boldsymbol{x_p} - \boldsymbol{dx_p}) - b_i = 0, \forall i, \\ \boldsymbol{W}^T (\boldsymbol{x_p} - \boldsymbol{dx_p}) - \boldsymbol{b} = \boldsymbol{0} &\Rightarrow \boldsymbol{W}^T (\boldsymbol{x_p} - \hat{\boldsymbol{S}} \boldsymbol{v_p}) - \boldsymbol{b} = \boldsymbol{0} \Rightarrow \\ \boldsymbol{W}^T \hat{\boldsymbol{S}} \boldsymbol{v_p} = \boldsymbol{W}^T \boldsymbol{x_p} - \boldsymbol{b} &\Rightarrow \boldsymbol{v_p} = (\boldsymbol{W}^T \hat{\boldsymbol{S}})^+ (\boldsymbol{W}^T \boldsymbol{x_p} - \boldsymbol{b}) \Rightarrow \end{aligned} \tag{10}$$

$$\boldsymbol{dx_p} = \hat{\boldsymbol{S}} \boldsymbol{v_p} = \hat{\boldsymbol{S}} (\boldsymbol{W}^T \hat{\boldsymbol{S}})^+ (\boldsymbol{W}^T \boldsymbol{x_p} - \boldsymbol{b}) \tag{11}$$

These manipulations are carried out for all $\boldsymbol{p}$ in the image representation $\boldsymbol{X}$ simultaneously, leading to a manipulated image representation $\boldsymbol{X'} = g(\boldsymbol{X}; \boldsymbol{W})$ or $\boldsymbol{X'} = h(\boldsymbol{X}; \boldsymbol{W}, \hat{\boldsymbol{S}})$, based on the manipulation type (Fig. 5).

Finally, the **Uncertainty Region Alignment Loss** ($\mathcal{L}^{ur}$) is:

$$\mathcal{L}^{ur} = -\mathbb{E}_{\boldsymbol{X'}} \big[\mathcal{H}(f^+(\boldsymbol{X'}) \big] \tag{12}$$

with $\mathcal{H}$ denoting entropy and f^+ denoting the part of the network after the layer of study that provides output class probabilities. When we manipulate the representations via either UFM or CFM, we use the layer's activation function (typically a ReLU) to keep the features in the input domain of the next layer. Throughout the experiments, we will denote Uncertainty Region Alignment loss with UFM as $\mathcal{L}^{uur}$ and with CFM as $\mathcal{L}^{cur}$. We consider the use of $\mathcal{L}^{uur}$ and $\mathcal{L}^{cur}$ to be mutually-exclusive. We either use the first or the second type of manipulation when computing the Uncertainty Region Alignment Loss and never both types at the same time.

4.5 Augmented Lagrangian Loss for Effective Direction Learning

Most of the loss terms that we use in our method are highly antagonistic. For example, concept detectors can make more confident predictions ($\mathcal{L}^{ma}$) when the separation margin ($\mathcal{L}^{mm}$) between positive and negative samples is small (while we seek to maximize it). In our experiments, we also observed that a high separation margin is also antagonistic to the sparsity of the clustering ($\mathcal{L}^s$ or $\mathcal{L}^{fs}$). Therefore, if we linearly combine the loss terms, the implementation of our approach across various network architectures and datasets necessitates meticulous adjustment of the loss weights within the objective function. The latter can be particularly laborious and time-consuming. Additionally, adjusting the loss weights only indirectly controls the quality of the clustering, as the final loss values can vary significantly with different weight sets. For these reasons, we choose a different strategy to learn our direction pairs. We base our method on ϵ-constrained optimization, formulating our objective as a minimization problem with inequality constraints. We use the Augmented Lagrangian formulation (Hestenes, 1969; Bertsekas, 2014) to solve the following optimization problem:

$$\min \quad \lambda^{fs}\mathcal{L}^{fs} + \lambda^{ur}\mathcal{L}^{ur} \quad s.t. \quad \begin{cases} \mathcal{L}^{ma} \leq \tau^{ma} \\ \mathcal{L}^{ic} \leq \tau^{ic} \\ \mathcal{L}^{mm} \leq \tau^{mm} \\ \mathcal{L}^{eac} \leq \tau^{eac} \\ \mathcal{L}^{fso} \leq \tau^{fso} \\ \mathcal{L}^{cs} \leq \tau^{cs} \end{cases} \tag{13}$$

with $\lambda^{fs}, \lambda^{ur} \in \mathbb{R}^+$ the only loss weight coefficients. In this formulation, we assign a target value τ to each individual loss term participating in the inequalities and, as shown in the experiments, subsequently optimize for interpretability ($\mathcal{L}^{fs}, \mathcal{L}^{uur}$), or a balance between interpretability $\mathcal{L}^{fs}$ and influence $\mathcal{L}^{cur}$.

5 Encoding-Decoding Direction Pairs in Applications

Moving forward to the application level, in this Section we discuss how to read concept information from the embeddings, how to intervene on the encoding of concepts (Section 5.1) and how to capitalize on the learned direction pairs to obtain local, detailed, and spatially-aware concept explanations (Section 5.2).

5.1 Reading Concept Information and Intervening on their Encoding

Reading Concept Information from the Embeddings Reading concept information from a patch embedding ends up in estimating the concept's signal value that is encoded in the representation. Supposing that the related conditions are met, in Section 3.2 it was shown that the filter direction can serve as a means to extract this value. While in the data-model of Section 3.2, the extraction of the signal's value is exact, under the multi-concept signal-distractor data model of Section 4.1 the considered latent space bias $\boldsymbol{c}$ is interfering with this value. More specifically, if we suppose $\boldsymbol{w}_i : \boldsymbol{w}_i \perp \hat{\boldsymbol{s}}_j, i \neq j, \boldsymbol{w}_i^T \hat{\boldsymbol{s}}_i = 1$ and $\boldsymbol{w}_i \perp \boldsymbol{D}$, the inner product between the filter and the embedding results in:

$$\boldsymbol{w}_i^T \boldsymbol{x}_{\boldsymbol{p}} = \alpha_{\boldsymbol{p},i} \underbrace{\boldsymbol{w}_i^T \hat{\boldsymbol{s}}_i}_{=1} + \boldsymbol{w}_i^T \boldsymbol{c} \Rightarrow \boldsymbol{w}_i^T \boldsymbol{x}_{\boldsymbol{p}} = \alpha_{\boldsymbol{p},i} + \underbrace{\boldsymbol{w}_i^T \boldsymbol{c}}_{const} \tag{14}$$

Thus, when considering our extended data model, the filter can be used to extract the signal's value but with an offset that is constant, regardless of $\boldsymbol{x}_{\boldsymbol{p}}$. Due to the offset being constant, the difference between two projected embeddings is equal to the difference of their signal values, e.g.:

$$\boldsymbol{w}_i^T (\boldsymbol{x}_{\boldsymbol{p}_1} - \boldsymbol{x}_{\boldsymbol{p}_2}) = \alpha_{\boldsymbol{p}_1,i} + \boldsymbol{w}_i^T \boldsymbol{c} - \alpha_{\boldsymbol{p}_2,i} - \boldsymbol{w}_i^T \boldsymbol{c} = \alpha_{\boldsymbol{p}_1,i} - \alpha_{\boldsymbol{p}_2,i} \tag{15}$$

In applications, we can exploit this property to estimate the signal value that is encoded in a patch embedding with respect to another patch embedding of reference. We found that two reference points are of particular interest. First, the average embedding over a collection of embeddings. In that case, we can estimate the signal value of $\boldsymbol{x}_{\boldsymbol{p}}$ with respect to the average signal value in the collection:

$$\boldsymbol{w}_i^T \boldsymbol{x}_{\boldsymbol{p}} - \boldsymbol{w}_i^T \mathbb{E}_{\boldsymbol{p}}\big[\boldsymbol{x}_{\boldsymbol{p}}\big] = \boldsymbol{w}_i^T \boldsymbol{x}_{\boldsymbol{p}} - \mathbb{E}_{\boldsymbol{p}}\big[\boldsymbol{w}_i^T \boldsymbol{x}_{\boldsymbol{p}}\big] = \alpha_{\boldsymbol{p},i} - \mathbb{E}_{\boldsymbol{p}}\big[\alpha_{\boldsymbol{p},i}\big] \tag{16}$$

And second, the concept's point of uncertainty. Given a query point $\boldsymbol{x}_{\boldsymbol{p}}$, the concept's point of uncertainty $\hat{\boldsymbol{u}}_{\boldsymbol{p}}$ is the point that lies on the concept detector's hyperplane (thus corresponds to a point of maximum concept ambiguity) and the line that is defined by the query point and the direction of the signal vector. More specifically, the point of uncertainty is equal to $\hat{\boldsymbol{u}}_{\boldsymbol{p}} = \boldsymbol{x}_{\boldsymbol{p}} - \kappa_{\boldsymbol{p},i}\hat{\boldsymbol{s}}_i$ with $\kappa_{\boldsymbol{p},i} \in \mathbb{R}$ corresponding to the solution of the following system of equations:

$$\left.\begin{array}{l}\hat{\boldsymbol{u}}_{\boldsymbol{p}} = \boldsymbol{x}_{\boldsymbol{p}} - \kappa_{\boldsymbol{p},i}\hat{\boldsymbol{s}}_i \\ \boldsymbol{w}_i^T\hat{\boldsymbol{u}}_{\boldsymbol{p}} - b_i = 0\end{array}\right\} \Rightarrow \boldsymbol{w}_i^T\hat{\boldsymbol{u}}_{\boldsymbol{p}} - b_i = 0 \Rightarrow \boldsymbol{w}_i^T(\boldsymbol{x}_{\boldsymbol{p}} - \kappa_{\boldsymbol{p},i}\hat{\boldsymbol{s}}_i) - b_i = 0 \Rightarrow \kappa_{\boldsymbol{p},i} = \frac{\boldsymbol{w}_i^T\boldsymbol{x}_{\boldsymbol{p}} - b_i}{\underbrace{\boldsymbol{w}_i^T\hat{\boldsymbol{s}}_i}_{=1}} = \boldsymbol{w}_i^T\boldsymbol{x}_{\boldsymbol{p}} - b_i \tag{17}$$

Typically $\hat{\boldsymbol{u}}_{\boldsymbol{p}}$ depends on i, but we drop this index for brevity. What is interesting about the point of uncertainty is that the following difference corresponds to centering the signal value of $\boldsymbol{x}_{\boldsymbol{p}}$ around the value that represents uncertainty:

$$\boldsymbol{w}_i^T\boldsymbol{x}_{\boldsymbol{p}} - \boldsymbol{w}_i^T\hat{\boldsymbol{u}}_{\boldsymbol{p}} = \boldsymbol{w}_i^T\boldsymbol{x}_{\boldsymbol{p}} - \boldsymbol{w}_i^T(\boldsymbol{x}_{\boldsymbol{p}} - \kappa_{\boldsymbol{p},i}\hat{\boldsymbol{s}}_i) = \kappa_{\boldsymbol{p},i}\underbrace{\boldsymbol{w}_i^T\hat{\boldsymbol{s}}_i}_{=1} = \kappa_{\boldsymbol{p},i} = \boldsymbol{w}_i^T\boldsymbol{x}_{\boldsymbol{p}} - b_i \tag{18}$$

Since (18) corresponds to the function of the concept detector, this difference is positive whenever the concept is present in $\boldsymbol{x}_{\boldsymbol{p}}$ and negative whenever the concept is absent. Thus, centering the signal value of a patch embedding around its point of uncertainty can be simply done by computing $\kappa_{\boldsymbol{p},i}$ using (17).

Intervening on Concept Encoding Altering the concept content that is encoded in a patch embedding ends up overwriting the signal value of the concept with a target value of interest. The target value is meant to be copied from a target embedding. Let $\boldsymbol{x}_{\boldsymbol{p}}$ denote the patch embedding that we aim to intervene on and $\boldsymbol{x}_{\boldsymbol{p}}^t$ denote the target embedding. Let $\boldsymbol{x}_{\boldsymbol{p}}'$ denote the altered embedding after the intervention. Supposing that we aim to intervene on the value of concept i, $\boldsymbol{x}_{\boldsymbol{p}}'$ becomes:

$$\boldsymbol{x}_{\boldsymbol{p}}' = \boldsymbol{x}_{\boldsymbol{p}} + \kappa_{\boldsymbol{p},i}\hat{\boldsymbol{s}}_i \tag{19}$$

with $\kappa_{\boldsymbol{p},i} \in \mathbb{R}$. Since we want $\boldsymbol{x}_{\boldsymbol{p}}'$ and $\boldsymbol{x}_{\boldsymbol{p}}^t$ to have the same signal value for concept i, we make use of (15) and compute $\kappa_{\boldsymbol{p},i}$ such that:

$$\boldsymbol{w}_i^T(\boldsymbol{x}_{\boldsymbol{p}}' - \boldsymbol{x}_{\boldsymbol{p}}^t) = 0 \Rightarrow \boldsymbol{w}_i^T(\boldsymbol{x}_{\boldsymbol{p}} + \kappa_{\boldsymbol{p},i}\hat{\boldsymbol{s}}_i - \boldsymbol{x}_{\boldsymbol{p}}^t) = 0 \Rightarrow \kappa_{\boldsymbol{p},i} = \frac{\boldsymbol{w}_i^T\boldsymbol{x}_{\boldsymbol{p}}^t - \boldsymbol{w}_i^T\boldsymbol{x}_{\boldsymbol{p}}}{\underbrace{\boldsymbol{w}_i^T\hat{\boldsymbol{s}}_i}_{=1}} = \underbrace{\boldsymbol{w}_i^T\boldsymbol{x}_{\boldsymbol{p}}^t}_{t} - \boldsymbol{w}_i^T\boldsymbol{x}_{\boldsymbol{p}} = t - \boldsymbol{w}_i^T\boldsymbol{x}_{\boldsymbol{p}} \tag{20}$$

with t denoting the projected target value. In applications, we are typically interested in altering the concept content of an embedding towards the presence or absence of a concept. To accomplish that, two natural choices arise: first, to overwrite the signal value of the embedding based on the average signal value of samples with or without the concept, and second, to overwrite the signal value of the embedding to match the value of a top (or bottom) quantile of signal values in a collection. In the first case, we can use $\boldsymbol{x}_{\boldsymbol{p}}^t = \mathbb{E}_p\big[\boldsymbol{x}_{\boldsymbol{p}}\big]$, with the average taking place along the patches with (or without) the concept. For the second case, we can directly work in the projection space, by computing the quantile of interest over the projected embeddings $\boldsymbol{w}_i^T\boldsymbol{x}_{\boldsymbol{p}}$ and use that value in place of t.

5.2 Using Encoding-Decoding Direction Pairs and the Regions of Uncertainty to Provide Concept-Based Local Explanations and Detailed Spatially-Aware Concept Contribution Maps

In this Section, we discuss how our learned Encoding-Decoding Direction Pairs can be leveraged in order to provide concept-based local explanations for any network prediction. For simplicity, we will be discussing the application in Convolutional Neural Networks (CNNs) with a Global Average Pooling (GAP) layer and a ReLU activation function, but adaptation to other architectures could be possible.

5.2.1 Terminology and Definitions

Suppose that we want to explain the prediction of an image classifier f for image $\mathcal{I}$. Let $\boldsymbol{X}$ denote this image's representation at the penultimate layer of the network (in CNNs, this is typically the last convolutional layer before GAP). Let also $\boldsymbol{x_p} \in \mathbb{R}^D$ denote a patch embedding in $\boldsymbol{X}$ at the spatial location $\boldsymbol{p} = (w, h)$. Following the previously introduced methodology, we assume that we have learned Encoding-Decoding Direction Pairs for this layer, i.e. filters $\boldsymbol{W}$ and signal vectors $\hat{\boldsymbol{S}}$. Let $l_c \in \mathbb{R}$ denote the network's output logit for class c regarding input $\mathcal{I}$. Typically, c will be chosen such that l_c is the maximum logit among the output class logits, but other choices are also valid, for instance when we want to explain why the prediction deviated from a specific class. Let also $\boldsymbol{X}_b^m \in \mathbb{R}^{H\times W\times D}$ denote a **baseline** point in the **uncertainty region of the model**. We call it baseline because this point corresponds to an artificial image representation for which the prediction of the network is highly uncertain. Let $l_b^m \in \mathbb{R}$ denote the prediction logit for class c that corresponds to $\boldsymbol{X}_b^m$, i.e. $l_b^m = f^+(\boldsymbol{X}_b^m)$. We define the following quantity:

$$l_e = l_c - l_b^m \tag{21}$$

an explanation logit (l_e), which is equal to the difference in predicting class c for image $\mathcal{I}$ compared to a highly uncertain prediction for the same class. Let $\boldsymbol{w}_c$ and b_c denote the class vector and the corresponding bias of the network's **last** fully connected layer. Then, the explanation logit becomes:

$$l_e = l_c - l_b^m = \boldsymbol{w}_c^T \mathrm{GAP}(\boldsymbol{X}) + b_c - (\boldsymbol{w}_c^T \mathrm{GAP}(\boldsymbol{X}_b^m) + b_c) \tag{22}$$

Our goal is to express this quantity in terms of the identified concepts. Based on our previous discussions in Sections 4.4 and 5.1, we conclude that an intuitive point of reference for expressing concept content is a **baseline point in the uncertainty region of the concept detectors**. Any image representation $\boldsymbol{X}$ has a corresponding **baseline** point $\boldsymbol{X}_b^c \in \mathbb{R}^{H\times W\times D}$ in that region, which can be obtained by $h(\boldsymbol{X}; \boldsymbol{W}, \hat{\boldsymbol{S}})$. If it weren't for the layer's activation function, we could choose $\boldsymbol{X}_b^m$ to be equal to $\boldsymbol{X}_b^c$, due to the alignment of the two uncertainty regions during direction learning. However, in practice, there is a shift between the two points, since $\boldsymbol{X}_b^m = \mathrm{ReLU}(\boldsymbol{X}_b^c)$. For this reason, we treat $\boldsymbol{X}_b^m$ similar to $\boldsymbol{X}$, i.e. as an artificial image representation whose concept content can be expressed with respect to a baseline point $\boldsymbol{X}_b^{mc}$ in the **uncertainty region of the concept detectors**. Similar to $\boldsymbol{X}_b^c$, $\boldsymbol{X}_b^{mc}$ can be calculated by $h(\boldsymbol{X}_b^m; \boldsymbol{W}, \hat{\boldsymbol{S}})$. Finally, let $\boldsymbol{v_p}$ and $\boldsymbol{v_p^b}$ be equal to the expression of (10) when computing baseline points in the concept detectors' uncertainty region for $\boldsymbol{X}$ and $\boldsymbol{X}_b^m$, respectively.

5.2.2 Logit Difference Decomposition in terms of Concepts

Based on the aforementioned definitions, we have:

$$\begin{aligned} l_e = l_c - l_b^m = \boldsymbol{w}_c^T \mathrm{GAP}(\boldsymbol{X}) + b_c - (\boldsymbol{w}_c^T \mathrm{GAP}(\boldsymbol{X}_b^m) + b_c) \Rightarrow \\ l_e = \boldsymbol{w}_c^T \mathrm{GAP}(\boldsymbol{X} - \boldsymbol{X}_b^c) - \boldsymbol{w}_c^T \mathrm{GAP}(\boldsymbol{X}_b^m - \boldsymbol{X}_b^{mc}) + \boldsymbol{w}_c^T \mathrm{GAP}(\boldsymbol{X}_b^c - \boldsymbol{X}_b^{mc}) \end{aligned} \tag{23}$$

Due to the linearity of GAP, (23) can be written as:

$$l_e = \mathbb{E}_{\boldsymbol{p}}\Big[\boldsymbol{w}_c^T(\boldsymbol{x_p} - \boldsymbol{x}_{\boldsymbol{p},b}^c)\Big] - \mathbb{E}_{\boldsymbol{p}}\Big[\boldsymbol{w}_c^T(\boldsymbol{x}_{\boldsymbol{p},b}^m - \boldsymbol{x}_{\boldsymbol{p},b}^{mc})\Big] + \mathbb{E}_{\boldsymbol{p}}\Big[\boldsymbol{w}_c^T(\boldsymbol{x}_{\boldsymbol{p},b}^c - \boldsymbol{x}_{\boldsymbol{p},b}^{mc})\Big] \tag{24}$$

where $\boldsymbol{x}_{\boldsymbol{p},b}^c, \boldsymbol{x}_{\boldsymbol{p},b}^m$ and $\boldsymbol{x}_{\boldsymbol{p},b}^{mc}$ elements at the spatial location $\boldsymbol{p}$ of $\boldsymbol{X}_b^c, \boldsymbol{X}_b^m$ and $\boldsymbol{X}_b^{mc}$, respectively. By definition, we have $\boldsymbol{x_p} - \boldsymbol{x}_{\boldsymbol{p},b}^c = \hat{\boldsymbol{S}}\boldsymbol{v_p}$, and $\boldsymbol{x}_{\boldsymbol{p},b}^m - \boldsymbol{x}_{\boldsymbol{p},b}^{mc} = \hat{\boldsymbol{S}}\boldsymbol{v_p^b}$, $\boldsymbol{v_p}, \boldsymbol{v_p^b} \in \mathbb{R}^I$. Given these, (24) can be written as:

$$l_e = \mathbb{E}_{\boldsymbol{p}}\Big[\boldsymbol{w}_c^T \hat{\boldsymbol{S}}(\boldsymbol{v_p} - \boldsymbol{v_p^b})\Big] + \mathbb{E}_{\boldsymbol{p}}\Big[\boldsymbol{w}_c^T \boldsymbol{r_p}\Big] \tag{25}$$

with $\boldsymbol{r_p} = \boldsymbol{x}_{\boldsymbol{p},b}^c - \boldsymbol{x}_{\boldsymbol{p},b}^{mc} \in \mathbb{R}^D$ a residual that is not going to be explained in terms of concepts. The first part of (25) can be interpreted as follows: the contribution of concept i to the explanation logit is equal to $\boldsymbol{w}_c^T \hat{\boldsymbol{s}}_i(v_{\boldsymbol{p},i} - v_{\boldsymbol{p},i}^b)$. This means that the explanation logit depends on a global concept contribution factor $\boldsymbol{w}_c^T \hat{\boldsymbol{s}}_i$ which is constant regardless of the sample to be explained, and a local contribution factor which depends on the sample and is equal to the difference in concept content between the sample itself and a synthetic baseline sample that corresponds to a highly uncertain network prediction. Since both $\boldsymbol{x}_{\boldsymbol{p},b}^c$ and $\boldsymbol{x}_{\boldsymbol{p},b}^{mc}$ lie in the uncertainty region of the concept detectors, their difference in terms of concept content is zero, and the residual does not carry any concept-related information.

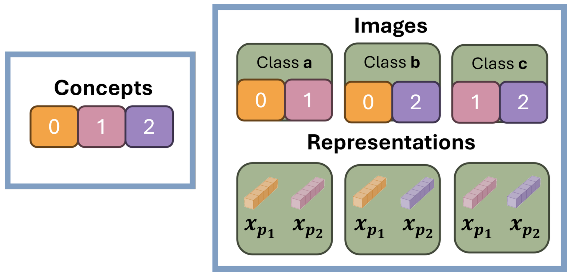

Figure 7: Description of the synthetic dataset that we use in the experiments: a) Concept set: $\{\mathbf{0,1,2}\}$ b) Image Classes: $\{\mathbf{a,b,c}\}$ with each class corresponding to a unique pair of concepts. c) Each image is comprised of two patch representations $\boldsymbol{x}_{\boldsymbol{p}_1}, \boldsymbol{x}_{\boldsymbol{p}_2}$.

Let $\hat{v}_{\boldsymbol{p},i}$ ($\hat{v}^b_{\boldsymbol{p},i}$) denote the signal value of $\boldsymbol{x}_{\boldsymbol{p}}$ ($\boldsymbol{x}^m_{\boldsymbol{p},b}$) for concept i centered around the value corresponding to the concept ambiguity (i.e. by considering $\boldsymbol{x}_{\boldsymbol{p}}$ ($\boldsymbol{x}^m_{\boldsymbol{p},b}$) as a query point and using the concept's point of uncertainty as a reference). As discussed in Section 5.1, positive $\hat{v}_{\boldsymbol{p},i}$ ($\hat{v}^b_{\boldsymbol{p},i}$) indicates concept presence, while negative $\hat{v}_{\boldsymbol{p},i}$ ($\hat{v}^b_{\boldsymbol{p},i}$) indicates concept absence. $\hat{v}_{\boldsymbol{p},i}$ ($\hat{v}^b_{\boldsymbol{p},i}$) and $v_{\boldsymbol{p},i}$ ($v^b_{\boldsymbol{p},i}$) would be exactly the same if $\boldsymbol{w}_i^T \hat{\boldsymbol{s}}_j = 0 \,\forall\, i \neq j$ and also if each $\boldsymbol{w}_i$ is perpendicular to the basis of distractors $\boldsymbol{D}$. In practice, these orthogonality constraints are only approximately fulfilled. To obtain intuitive explanations without compromising fidelity, we re-write (25) as:

$$l_e = \mathbb{E}_{\boldsymbol{p}}\Big[\boldsymbol{w}_c^T \hat{\boldsymbol{S}}(\hat{\boldsymbol{v}}_{\boldsymbol{p}} - \hat{\boldsymbol{v}}^b_{\boldsymbol{p}}) + \boldsymbol{w}_c^T \hat{\boldsymbol{S}}(\boldsymbol{v}_{\boldsymbol{p}} - \hat{\boldsymbol{v}}_{\boldsymbol{p}} - (\boldsymbol{v}^b_{\boldsymbol{p}} - \hat{\boldsymbol{v}}^b_{\boldsymbol{p}})\Big] + \mathbb{E}_{\boldsymbol{p}}\Big[\boldsymbol{w}_c^T \boldsymbol{r}_{\boldsymbol{p}}\Big] \Rightarrow \tag{26}$$

$$l_e = \underbrace{\mathbb{E}_{\boldsymbol{p}}\Big[\boldsymbol{w}_c^T \hat{\boldsymbol{S}} \hat{\boldsymbol{v}}_{\boldsymbol{p}}\Big]}_{\text{sample concept}} - \underbrace{\mathbb{E}_{\boldsymbol{p}}\Big[\boldsymbol{w}_c^T \hat{\boldsymbol{S}} \hat{\boldsymbol{v}}^b_{\boldsymbol{p}}\Big]}_{\text{baseline concept}} + \underbrace{\mathbb{E}_{\boldsymbol{p}}\Big[\boldsymbol{w}_c^T \hat{\boldsymbol{S}}(\boldsymbol{v}_{\boldsymbol{p}} - \hat{\boldsymbol{v}}_{\boldsymbol{p}} - (\boldsymbol{v}^b_{\boldsymbol{p}} - \hat{\boldsymbol{v}}^b_{\boldsymbol{p}})\Big]}_{\text{correction}} + \underbrace{\mathbb{E}_{\boldsymbol{p}}\Big[\boldsymbol{w}_c^T \boldsymbol{r}_{\boldsymbol{p}}\Big]}_{\textit{residual}} \tag{27}$$

Based on (27), the explanation logit l_e is linearly expressed in terms of patches and concepts, giving detailed, spatially-aware information for concept contributions. We split (27) into four parts. The first part corresponds to contributions of concepts included in the sample (*sample concept*), the second to the contribution of concepts contained in an artificial baseline point of an uncertain prediction (*baseline concept*), the third part to a *correction* factor to account for imperfect direction learning convergence, and finally a *residual* that we do not explain. If the correction factor for concept i was zero, concept i would have a positive contribution to the explanation logit whenever the difference in contributions between the sample and the baseline is positive. In the case of imperfect learning conditions, this difference must exceed the negative of the correction factor.

In the experiments, we will be reporting Concept Contribution Maps (CCMs) where each spatial element $\boldsymbol{p}$ will be equal to:

$$\phi^i_{\boldsymbol{p}} = \boldsymbol{w}_c^T \hat{\boldsymbol{s}}_i (\hat{v}_{\boldsymbol{p},i} - \hat{v}^b_{\boldsymbol{p},i}) \tag{28}$$

visualized as a heatmap over the original image for a given concept i. Finally, we will be referring to the quantity $\boldsymbol{w}_c^T \hat{\boldsymbol{s}}_i$ as the Concept-Class Relation Coefficient (CCRC).

6 Experiment on Synthetic Data

In this section, we test our method on synthetic data which follow the data generation process detailed in Section 4.1. We validate three aspects: a) the effectiveness of signal vectors in estimating the concept's encoding direction **given ground-truth signal values**, b) the efficacy of our **unsupervised** approach to reliably identify the ground-truth concept encoding-decoding direction pairs, under challenging conditions for conventional techniques, c) the necessity of Filter-Signal Orthogonality loss $\mathcal{L}^{fso}$ for reliable estimation of encoding directions.

We consider synthetic **image representations** with two spatial elements $\boldsymbol{p}_1, \boldsymbol{p}_2$, i.e. $W = 2$ and $H = 1$. Every pixel $\boldsymbol{p}$ is presumed to be associated with just one concept from a set of $I = 3$ concepts. Let

Table 1: Evaluating the performance of the concept detectors in classifying patch embeddings in the experiment on synthetic data. The metric is Intersection over Union (IoU). Rows correspond to concept detectors and columns to ground-truth concept classes. Clearly, each detector is aligned with one distinct ground-truth concept.

		Concept		
		#0	**#1**	**#2**
Detector	**#0**	0	1.0	0
	#1	1.0	0	0
	#2	0	0	1.0

$c(\boldsymbol{p}) \in \{0, 1, 2\}$ represent the concept label of $\boldsymbol{p}$, and $k \in \{a, b, c\}$ denote an image class. We construct **image representations** as follows: for $k = a$, $c(\boldsymbol{p}_1) = 0$ and $c(\boldsymbol{p}_2) = 1$; for $k = b$, $c(\boldsymbol{p}_1) = 0$ and $c(\boldsymbol{p}_2) = 2$; and for $k = c$, $c(\boldsymbol{p}_1) = 1$ and $c(\boldsymbol{p}_2) = 2$ (Fig. 7). We set the embedding space dimensionality to $D = 8$, the size of the distractor basis to $F = 2$ and randomly create unit-norm vectors to construct the matrices $\boldsymbol{S}$ and $\boldsymbol{D}$. Using those principles and hyper-parameters we generate **patch embeddings** $\boldsymbol{x}_{\boldsymbol{p}_1}, \boldsymbol{x}_{\boldsymbol{p}_2}$ for each image according to (3). The latent signal values and distractor coefficients follow the uniform distribution: $\alpha_{\boldsymbol{p},i} \sim \mathcal{U}(0.0, 2.25)$ if $\boldsymbol{p}$ is not part of concept i and $\alpha_{\boldsymbol{p},i} \sim \mathcal{U}(2.75, 5.0)$, otherwise, while $\beta_{\boldsymbol{p},f} \sim \mathcal{U}(0, 5.0)$ is independent of the patch's concept label. We introduce a bias of $\boldsymbol{c} = 10$ across all dimensions of the representations to maintain them in the positive quartile, similar to the impact of a ReLU layer. We generate a balanced dataset with each class being represented by 1000 images.

Given the aforementioned synthetic dataset, we train a network to predict the image class based on the concept content of its patches. The network we use is composed of just two layers (corresponding to the top part of a potentially larger deep network). The first is an average-pooling layer, and the second is a linear layer with $K = 3$ output classes. After training, the network attains 96.33% accuracy on a test set, randomly generated based on the previous principles. More details regarding the setup of this experiment are provided in Section A.4.

6.1 Evaluation of the Signal-Vector Estimator

Based on the synthetic pixel dataset $\{\boldsymbol{x}_{\boldsymbol{p}_1}\} \cup \{\boldsymbol{x}_{\boldsymbol{p}_2}\}$ and the **ground-truth signal values** $\alpha_{\boldsymbol{p},i}$ that we randomly generated, we put the estimator of Kindermans et al. (2017) and our signal vectors under test. The difference between the two estimators is the sub-sampling procedure that we proposed in Section 4.3. Given the ground-truth matrix of signal directions $\boldsymbol{S}$ we are able to calculate cosine similarities between the estimated signal directions and the respective ground-truth. The results of this experiment are depicted in Fig. 8 (in **blue** and **green**). Since we make use of the ground-truth signal values, this experiment evaluates the efficacy of signal vectors under perfect input conditions. The figure showcases the effectiveness of our proposed sub-sampling procedure when using (1) as in all cases signal vectors demonstrate perfect alignment with the ground-truth directions, while in the absence of sub-sampling, the estimation is less reliable. Conclusively, the sub-sampling technique that we proposed in Section 4.3 successfully adapts to the new assumptions that we make about the data.

6.2 Evaluation of the Encoding-Decoding Direction Pairs

In this experiment, signal vectors are jointly learned with the concept detectors in an unsupervised fashion, employing every proposed facet of the method as laid out in Section 4. Concept detectors are evaluated for their ability to detect each one of the ground-truth concepts, while signal vectors are evaluated for their alignment with the ground-truth concept encoding directions.

Decoding Directions (Concept Detectors): Using the synthetic pixel dataset $\{\boldsymbol{x}_{\boldsymbol{p}_1}\} \cup \{\boldsymbol{x}_{\boldsymbol{p}_2}\}$, we assess the ability of each learned concept detector in detecting each one of the ground-truth concepts. Since the method is unsupervised, the name of the concept that each detector detects is unknown. For this reason, we need to implement direction labeling (Section 3.4). In Table 1 we present the Intersection over Union scores for each detector against actual concept classes. Zero values indicate complete purity and no mixing of the

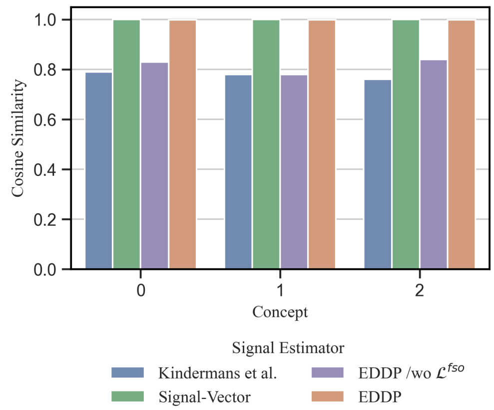

Figure 8: **1)** Cosine similarity between the ground-truth concept encoding directions and their estimation via Kindermans et al (1) calculated **without** our proposed feature sub-sampling. In this experiment, the estimation of signal directions **uses ground-truth signal values**. **2)** Cosine similarity between the ground-truth concept encoding directions and their estimation via Signal-Vectors, i.e. using (1) calculated **with** our proposed feature sub-sampling. Similarly to the previous experiment this one uses **ground-truth signal values**. Under ideal input conditions, Signal-Vectors are proven to be faithful signal estimators. **3)** Cosine similarity between ground-truth concept encoding directions and their estimation via our proposed Encoding-Decoding Direction Pairs (EDDP). In constrast to the previous two experiments, in this one Signal Vectors are learned in an **unsupervised** manner using all the aspects of the proposed method. Without access to ground-truth signal values, our overall unsupervised approach is capable of recovering the ground-truth concept encoding directions. **4)** Cosine similarity between the ground-truth concept encoding directions and their estimation via our proposed Encoding-Decoding Direction Pairs (EDDP). This experiment is identical to (3) but omits the Filter-Signal Orthogonality Loss $\mathcal{L}^{fso}$ from the objective function. In that case, the encoding direction estimation is inferior compared to when employing $\mathcal{L}^{fso}$.

concepts, while scores of 1.0 indicate perfect concept detection. As an additional step, we also examine how well the learned filters extract signal values from representations. Since distractors and the latent space bias $\boldsymbol{c}$ are not directly estimated by our method, we can only quantify the extracted signal values as a deviation from the dataset's average value (See also (16) and Section A.5). The Root Mean Squared Error (RMSE) between these extracted values and the ground truth, after subtracting the mean signal value, is noted as 0.06. We also verified that in this experiment where the distractor components are **independent** of the concept content contained in the features, the learned filters were orthogonal to all the vectors in the distractor basis $\boldsymbol{D}$, **without** explicitly enforcing this to happen.

Encoding Directions: Fig. 8 - **orange** indicates perfect alignment between the learned signal vectors and the ground-truth concept encoding directions. We stress the fact that in this experiment signal vectors were learned in an unsupervised manner together with the concept detectors, and this is different from the approach we took in Section 6.1, where we evaluated signal vectors as estimators under ideal input conditions.

6.3 Ablation Study

In this synthetic experiment we also consider a case study where we learn the direction pairs by omitting $\mathcal{L}^{fso}$ from the objective function, i.e. learning the direction pairs without (/wo) it. In that case, the concept detectors still discovered the ground-truth directional clusters, as in Table 1. However, the decoding directions were less reliable in extracting the ground-truth signal values. The RMSE between the extracted values and the ground truth, after subtracting the mean signal value, was found to be 0.31, which is substantially inferior to the standard case discussed above. The latter has an impact on the fidelity of the signal vectors. Fig. 8 **purple** visualizes the cosine similarity between the learned signal vectors and the ground-truth encoding directions for this case. The experiment shows that the signal direction estimation is less effective compared to when $\mathcal{L}^{fso}$ is taken into account.

6.4 Evaluation against other State-of-the-Art

The ground-truth encoding directions of this example (Table 14 in Appendix A.4) contain both positive and negative components, and the relationship among the encoding directions (and the distractors) is in general not orthogonal. In theory, and without the need for practical experiments, this example cannot be addressed by NMF, K-Means, or PCA. NMF would produce a signal basis of non-negative components. Similarly, the cluster centers of K-Means would point toward the positive quartile where the centroids reside. Finally, the non-orthogonal nature of the ground truth encoding directions implies that the PCA's solution space is insufficient.

7 Experiments on Deep Image Classifiers

In this section we apply our method in real-world scenarios. We perform a multifaceted analysis with the aim to shed light on every merit of the method, the method's relation to other supervised and unsupervised direction learning approaches, and finally its utility in real-world applications. In the following sections we a) assess the faithfulness of the learned encoding-decoding direction pairs b) provide qualitative segmentation results obtained by utilizing our learned concept detectors c) compare with the unsupervised state-of-the-art in interpretability and influence terms d) conduct an ablation study to quantify the contribution of each proposed component e) compare with supervised direction learning with the aim to provide more insights on the interpretability and influence of the directions f) provide application use cases in which the learned direction pairs assist in providing global, local and counterfactual model explanations g) provide an example application in model correction.

7.1 Direction Learning and Evaluation Protocol

We apply our Encoding-Decoding Direction Pairs (EDDP) on the last convolution layer of five different networks: ResNet18 (He et al., 2016) trained on Places365 (Zhou et al., 2017), ResNet50 (He et al., 2016) trained on Moments in Time (MiT) (Monfort et al., 2019) as well as EfficientNet (b0) (Tan & Le, 2019), Inception-v3 (Szegedy et al., 2016) and VGG16 (Simonyan & Zisserman, 2014) trained on ImageNet (Deng et al., 2009). For learning the direction pairs and quantitatively assessing their interpretability and their influence on network predictions, we expand on the protocol introduced in Doumanoglou et al. (2023). For all the networks that we study, when learning the direction pairs we use the Broden (Bau et al., 2017) concept dataset, except for ResNet50 for which we use Broden-Action Ramakrishnan et al. (2019). The concept datasets feature dense pixel annotations; Broden includes 1197 concepts across $63K$ images in 5 concept categories (*object, part, material, texture, color*), while Broden-Action incorporates an additional *action* category with 210 labels and $23K$ more images. We emphasize that when learning the direction pairs we do not make use of the annotations that complement the concept datasets.

For baselines, we consider directional clusterings based on either PCA, NMF, or the natural latent space basis. For our EDDP, we examine two variants, namely EDDP-U and EDDP-C. These are differentiated based on the choice of feature manipulation strategy used in Uncertainty Region Alignment, with EDDP-U referring to UFM and EDDP-C to CFM. Unless stated otherwise, our Encoding-Decoding Direction Pairs use the Augmented Lagrangian Loss from Section 4.5, all losses from Sections 4.2 and 3.3 (except $\mathcal{L}^s$), along with either $\mathcal{L}^{uur}$ (EDDP-U) or $\mathcal{L}^{cur}$ and $\mathcal{L}^{fso}$ (EDDP-C) from Sections 4.3 and 4.4. Other method parameters for each case are detailed in Section A.7. We emphasize that EDDP-U does not include the use of $\mathcal{L}^{fso}$ to learn the directions. We remind that the main purpose of $\mathcal{L}^{fso}$ is to contribute towards a faithful estimation of the encoding directions. While this was critical for the experiment on synthetic data, in real-world experiments, we see that the value of this loss is sufficiently low even when not directly minimizing it, possibly due to working in a high-dimensional embedding space where two random vectors are approximately orthogonal. A detailed discussion regarding $\mathcal{L}^{fso}$ is provided in Sections A.9 and A.10 with the conclusions presented in the main body of the article being mostly aligned with the conclusions that stem from detailed ablation studies.

After learning the directions, either with our method or with methods from the unsupervised state-of-the-art, we use the annotations available in the concept datasets to label the directions using Network Dissection

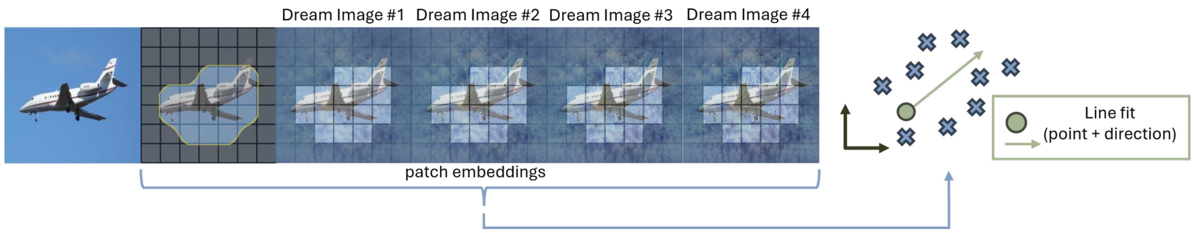

Figure 9: Our approach to assess the faithfulness of the direction pair: Starting from an image with the concept, we use deep dream to maximize the concept's decoding direction and collect, during "dreaming", the patch embeddings from the dream images at the regions with the concept. Subsequently, we fit a parametric line to those features in order to estimate the direction towards which they are moving when "dreaming". We term this direction as the *dreaming direction*.

(Bau et al., 2017). As described in Section 3.4, we make a basis change by projecting the network feature activations onto the learned decoding directions (for PCA and EDPP) or by directly utilizing the concept factors learned by NMF. While our approach is explicitly learning binary classifiers $\{\boldsymbol{w}_i, b_i\}$ as concept detectors, PCA and NMF lack the estimation of an explicit classification threshold b. To form concept detectors in those cases, we follow Bau et al. (2017) and for each direction we choose b to be equal to the top k-quantile among the projected activations sourced from the concept dataset. For NMF we use $k = 0.005$, as suggested in Bau et al. (2017), while for PCA we use $k = 0.2$ as suggested in Graziani et al. (2023a). In our experiments we also consider comparing with the clustering obtained using the natural latent space basis, i.e. the neuron directions, which in the tables we refer to as *Natural*. In that case, the classification threshold of the considered concept detectors is set to the top 0.005 quantile of the feature activations in the direction of the neuron, as originally suggested in Network Dissection.

7.2 Faithfulness Assessment of the Encoding-Decoding Direction Pairs

In this section, we aim to evaluate the faithfulness of the encoding-decoding direction pairs, i.e. to assess whether the signal value extracted by the decoding direction is indeed encoded in the direction of the signal vector. Although we already validated that the direction pairs are faithful in the case of synthetic data (Section 6), in this paragraph, we aim to make the same evaluation in the case of real data, in the absence of ground truth. Based on activation maximization (Nguyen et al., 2019), we propose the following novel approach to address this evaluation. Suppose that we evaluate the faithfulness of a particular direction pair $\boldsymbol{w}, \hat{\boldsymbol{s}}$ and let b denote the respective concept detector's bias. We use the concept detector $(\boldsymbol{w}, b)$ in order to collect a set of images containing the concept. Subsequently, using these images as an initialization point, we use Deep Dream (Olah et al., 2017) to compute *pre-images* (Mahendran & Vedaldi, 2015; 2016), that is, images that maximize the decoding direction $\boldsymbol{w}$ at the spatial locations of where the concept was initially found. In this manner, we start from an image containing the concept and ask Deep Dream to amplify (in the input pixel space) whatever concept the detector can detect. We keep running the activation maximization loop for K iterations and keep a record of how the features (at the locations with the concept) evolve while optimizing. Finally, we use all the recorded features collected during the "dreaming" optimization in order to fit a parametric line and estimate the direction that best describes feature evolvement while dreaming. We call the direction of this line *the dreaming direction* (Fig. 9). We conclude by comparing the dreaming direction of the concept for each image with the respective signal vector in terms of cosine similarity. In Figures 11 and 12 we provide histograms of these cosine similarities when applying our method to ResNet18 and EfficientNet. In all cases, even the ones without considering $\mathcal{L}^{fso}$, approximately 90% of the signal vectors have cosine similarity with the dreaming directions above 0.7, indicating sufficient faithfulness. The effect of $\mathcal{L}^{fso}$ is to push the distribution to become more Gaussian. To validate the effectiveness of the sub-sampling strategy proposed in Section 4.3 we also provide histograms of cosine similarities between signal vectors and dreaming directions in the absence of sub-sampling. The results are depicted in Fig. 13 where, in that case, the deviation of the signal vectors from the dreaming direction is evident. Example dreaming pre-images for two cases are provided in Fig. 10 and further details and experiments may be found in Sections A.6 and A.9.

Figure 10: Dreaming pre-images from the process of estimating the dreaming directions. **Left:** Maximizing a concept detector learned for the latent space of ResNet18 and labeled with the concept name *skyscraper*. **Right:** Maximizing a concept detector learned for the latent space of EfficientNet and labeled with the concept name *tvmonitor*. Both images regard directions learned with EDDP-C.

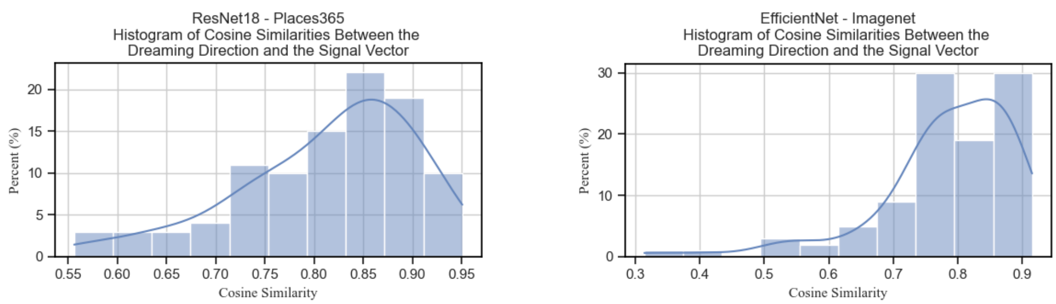

Figure 11: Cosine similarity histogram between *dreaming directions* and *signal vectors*. **Left:** Directions learned for ResNet18 trained on Places365 ($I = 448$). **Right**: Directions learned for EfficientNet trained on ImageNet ($I = 1120$). These histograms regard EDDP-C, i.e. directions learned **with** $\mathcal{L}^{cur}$ **and** $\mathcal{L}^{fso}$.

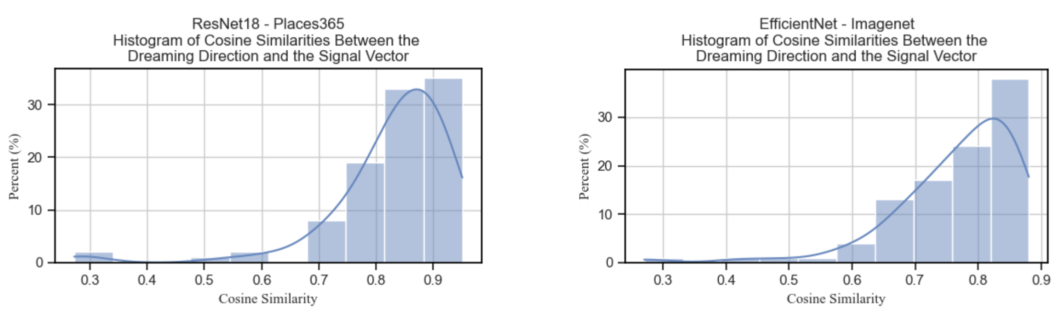

Figure 12: Cosine similarity histogram between *dreaming directions* and *signal vectors*. **Left:** Directions learned for ResNet18 trained on Places365 ($I = 448$). **Right**: Directions learned for EfficientNet trained on ImageNet ($I = 1120$). These histograms regard EDDP-U, i.e. directions learned with $\mathcal{L}^{uur}$ but **without** $\mathcal{L}^{fso}$.

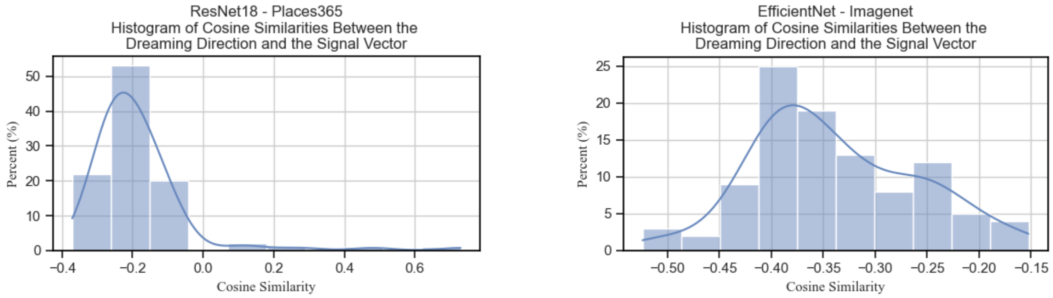

Figure 13: Cosine similarity histogram between *dreaming directions* and *signal vectors* learned **without sub-sampling**. **Left:** Directions learned for ResNet18 trained on Places365 ($I = 448$). **Right**: Directions learned for EfficientNet trained on ImageNet ($I = 1120$). These histograms regard EDDP-U, i.e. directions learned with $\mathcal{L}^{uur}$ but **without** $\mathcal{L}^{fso}$.

7.3 Interpretability Evaluation of Concept Detectors: Qualitative Segmentation Results and Interpretability Statistics

Figure 14 depicts qualitative segmentation results obtained using our concept detectors. Visualizations are obtained using Network Dissection (Bau et al., 2017). In the figures, the Intersection over Union (IoU) scores refer to the whole validation split of the concept dataset and not individual image segmentations. We can verify that concept detectors appear to be mostly monosemantic. For each network architecture, we additionally report interpretability statistics provided by Network Dissection. In this report, a concept detector is considered to be interpretable whenever its IoU performance with the best possible concept in the concept dataset exceeds the threshold of 0.04, which is equal to what was suggested in Network Dissection. Table 2 depicts this summary for ResNet18, while for the rest of the architectures, the results are summarized in Tables of the Appendix (Section A.12). More qualitative visualizations and visual comparisons with the unsupervised state-of-the-art are also included in the same Section of the Appendix.

Table 2: Network Dissection statistics for ResNet18 trained on Places365. For each concept category in Broden, we report two numbers: First, the number of concept detectors that were labeled with the name of a concept belonging to the category and second, the number of unique concept labels from the category that have been assigned to the set of the concept detectors. The table summarizes statistics for methods of the unsupervised state-of-the-art and for different values of the cluster count hyper-parameter I.

			ResNet18 / Places365					
I	**Method**	**Color**	**Object**	**Part**	**Material**	**Scene**	**Texture**	**Total**
384	PCA	0 / 0	22 / 13	5 / 2	1 / 1	28 / 16	117 / 32	173 / 64
	NMF	0 / 0	94 / 42	7 / 4	2 / 2	189 / 101	47 / 26	339 / 175
	EDDP-U	2 / 2	118 / 54	8 / 7	3 / 3	151 / 114	21 / 17	303 / 197
	EDDP-C	2 / 2	117 / 51	9 / 6	4 / 4	153 / 114	22 / 17	307 / 194
448	PCA	0 / 0	22 / 13	5 / 2	1 / 1	28 / 16	127 / 33	183 / 65
	NMF	0 / 0	95 / 46	9 / 7	1 / 1	234 / 120	33 / 20	372 / 194
	EDDP-U	2 / 2	137 / 62	6 / 6	5 / 5	193 / 129	21 / 18	364 / 222
	EDDP-C	2 / 2	136 / 60	5 / 5	5 / 5	194 / 133	22 / 18	364 / 223
512	Natural	0 / 0	107 / 43	11 / 8	1 / 1	269 / 135	26 / 17	414 / 204
	PCA	0 / 0	22 / 13	5 / 2	1 / 1	27 / 15	125 / 32	180 / 63
	EDDP-U	1 / 1	127 / 66	10 / 10	4 / 4	236 / 161	29 / 22	407 / 264
	EDDP-C	1 / 1	128 / 66	11 / 11	4 / 4	236 / 165	27 / 22	407 / 269

As an exemplar interpretation of the report, Table 2 shows that when learning direction pairs for ResNet18 with $I = 512$, Network Dissection reported that EDDP-C can identify 269 different concepts in the following categories: 66 objects, 165 scenes, 11 parts, 4 materials, 22 textures, and 1 color. The total number of interpretable concept detectors is 407. This preliminary statistical report together with the visualizations is given in order to provide an intuition regarding the interpretability of the concept detectors. A rigorous evaluation with comparisons is conducted in the Sections that follow.

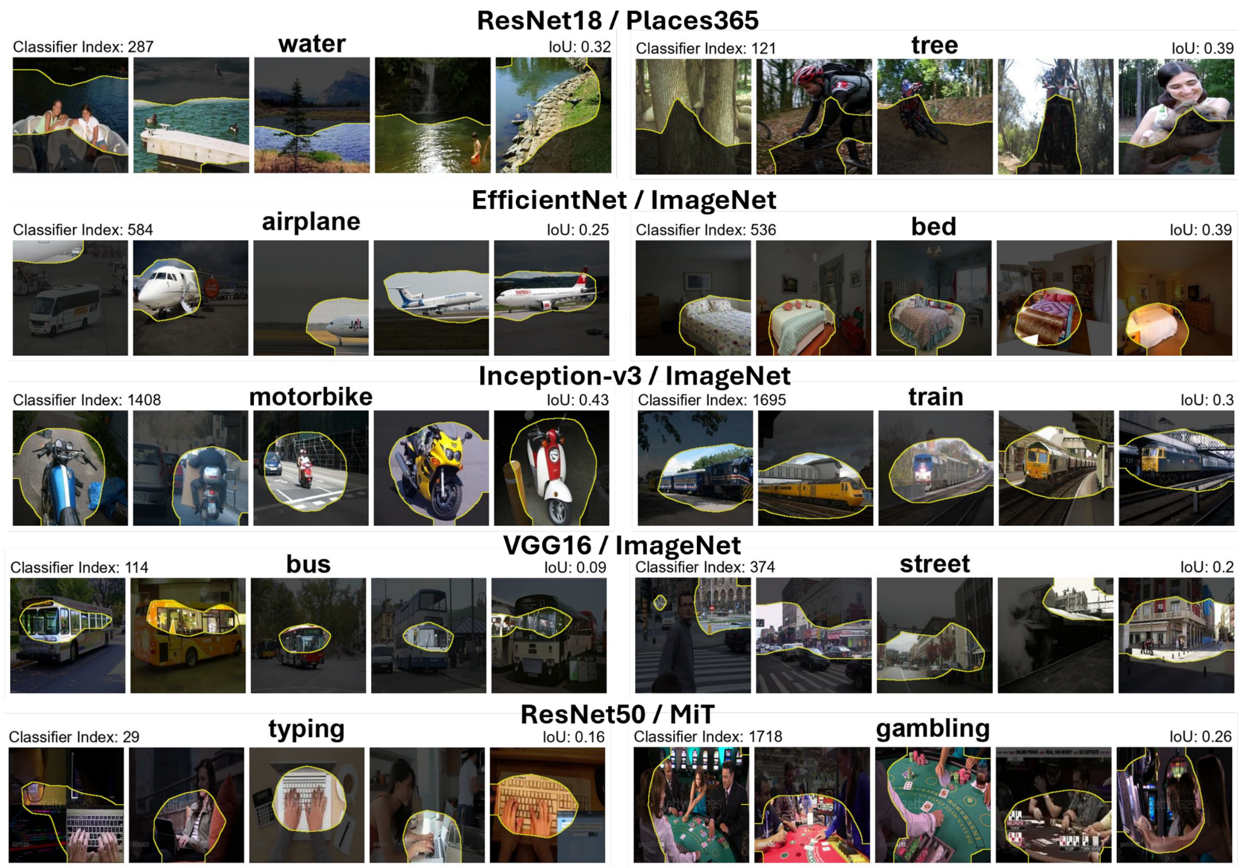

Figure 14: Qualitative segmentations using the concept detectors learned with our method as reported by Network Dissection. Rows correspond to concept detectors learned for different networks. For ResNet18 and EfficientNet the results were obtained using CFM while for Inception-v3, VGG16 and Resnet50 using UFM.

7.4 Metrics

7.4.1 Evaluation of Clustering Quality via Cluster Statistics

We report two statistical measures regarding the directional clustering. First, *Coverage* measures the percent of patches in the concept dataset that are classified positively by at least one of the concept detectors in the set, and second, *Redundancy* measures the average number of classifiers making a positive prediction for each patch in the dataset. *Coverage* may also be interpreted as the percent of pixels that have been assigned to at least one cluster, or the percent of pixels *explained* by the clustering, and *redundancy* may also be interpreted as the average number of clusters to which each patch belongs.

7.4.2 Evaluation of the Decoding Directions: Interpretability

Classification Let $\mathcal{T}_i$ denote the binary classification task of predicting whether a patch belongs to concept i. Given the concept label l which was assigned to a concept detector from Network Dissection, we assess the detector's performance on $\mathcal{T}_l$ using the standard binary classification metrics of Precision, Recall, F1, and Average Precision (AP). For each metric, we report average and standard deviation scores by aggregating across all detectors in the learned set.

Segmentation We additionally consider the performance of concept detectors in the binary semantic segmentation task and employ two metrics from Doumanoglou et al. (2023). Specifically, let $\phi_i(c, \mathcal{K})$ the Intersection Over Union for concept detector i in identifying concept c within the dataset $\mathcal{K}$. Define $c_i^\star = \text{argmax}_c \phi_i(c, \mathcal{K}_t)$, indicating the concept label detected best by concept detector i within the training subset of the dataset ($\mathcal{K}_t$). With $\mathcal{K}_v$ as the validation subset, we use the following interpretability scores $\mathcal{S}^1$ and $\mathcal{S}^2$:

$$\mathcal{S}^1 = \int_0^1 \sum_{i=0}^{I-1} \mathbb{1}_{x \geq \xi}\big(\phi_i(c_i^*, \mathcal{K}_v)\big) d\xi \tag{29}$$

$$\mathcal{S}^2 = \int_0^1 |\{c_i^\star \,|\, \exists\, i : \phi_i(c_i^\star, \mathcal{K}_v) \geq \xi\}| d\xi \tag{30}$$

The first metric $\mathcal{S}^1$ counts concept detectors with an IoU performance that exceeds a score threshold ξ. The second metric $\mathcal{S}^2$ uses the cardinality of the set $|.|$ to count the unique concept labels detected by the concept detectors with IoU above ξ. Both metrics become threshold-agnostic, by integrating on all $\xi \in [0, 1]$. Viewing it from a different angle, $\mathcal{S}^1$ pertains to the segmentation efficiency of each concept detector individually, whereas $\mathcal{S}^2$ concerns the **clustering diversity**, meaning the capability of the detector ensemble to recognize a wide array of distinct concepts. Finally, we also report the standard mean Intersection over Union (mIoU) score, which is the average IoU performance score aggregated across all the detectors in the set.

Monosemanticity Even though Precision is a natural classification metric that can capture the monosemanticity of the clustering, it has the drawback of relying on the explicit labels that are available in the concept dataset. To overcome this labeling limitation, and inspired by Dreyer et al. (2024b), we additionally quantify the monosemanticity of the concepts identified by the concept detectors by utilizing the embedding space of CLIP ViT/B-16 (Radford et al., 2021). In particular, for each concept detector, we pick images from the validation split of the concept dataset for which the detector is most confident about the presence of the concept. We pick 100 unique images from the top confident predictions. Subsequently, we crop a rectangle around the area of the concept and obtain the CLIP embedding for this crop. Let k_1^i and k_2^i denote image indices in the set of selected images with $k_1^i, k_2^i \in \{0, 1, ...99\}$ and i denote the i-th concept detector. We use the following monosemanticity metric, which measures the average distance between CLIP embeddings $(\boldsymbol{e}_{k_1^i}, \boldsymbol{e}_{k_2^i})$ within a cluster, aggregated over all clusters:

$$\mathcal{M} = \mathop{\mathbb{E}}_{i}\Big[\mathop{\mathbb{E}}_{k_1^i \neq k_2^i}\big[||\boldsymbol{e}_{k_1^i} - \boldsymbol{e}_{k_2^i}||_2\big]\Big] \tag{31}$$

7.4.3 Evaluation of the Encoding Directions: Influence

In the context of this evaluation, we relate concept influence to the sensitivity of the network with respect to that concept when making class predictions. We assess the ability of our method to identify influential concepts to model predictions using RCAV Pfau et al. (2020). As we already mentioned in Section 3.5, RCAV originally used CAVs to accomplish this. Here we follow the proposition of Pahde et al. (2024) and use the learned encoding directions in their place. For sensitivity scores, we spatially replicate the learned encoding directions across all spatial locations in the image representation. Direction significance is tested with RCAV's label permutation test to generate random directions, with the significance threshold set to 0.05 and Bonferroni correction. For RCAV's hyper-parameter α we use $\alpha = 5.0$, as originally suggested. In the ablation studies, two metrics summarize the results: Significant Direction Count (SDC) and Significant Class-Direction Pairs (SCDP). SDC represents the number of signal vectors that significantly influence at least one model class, while SCDP tallies class-direction pairs where the signal vectors significantly affect the class. In those metrics significance is measured by taking into account the influence of random directions on the network predictions as it was already discussed in Section 3.5. In studies without $\mathcal{L}^{cur}$, we report influence metrics for signal vectors that were estimated **post learning the directions** with the subsample strategy discussed in Section 4.3. Let also $S_{C,i,k}$ denote the sensitivity of the model to concept i when predicting class k (as measured by RCAV and scaled in the range $[-1.0, 1.0]$). When comparing against the unsupervised state-of-the-art, we use the following influence metric $\mathcal{I}^1$ which is defined as:

$$\mathcal{I}^1 = \mathbb{E}_{i,k}\Big[|S_{C,i,k}|\Big] \tag{32}$$

i.e. the average sensitivity of the model across all concepts and classes.

7.5 Interpretability and Influence Comparison with the Unsupervised State-of-the-Art

For comparing with the unsupervised state-of-the-art in direction learning, we consider baselines based on PCA and NMF which have been previously used in Zhang et al. (2021); Fel et al. (2023c) and Graziani et al. (2023a;b). While these previous works have demonstrated the effectiveness of PCA and NMF to reveal interpretable directions in the latent space of deep networks, their evaluation mostly relied on subjective human experiments. Going beyond subjective evaluation, in this work, we take a best effort approach to compare them with our method in quantitative terms of interpretability and influence. In the Appendix (Section A.11), we also compare with the methods we extend (Doumanoglou et al., 2023; 2024) but under a different protocol for a fair comparison. For each network, we consider three sizes for the clustering, namely $I = 3/4D$, $I = 7/8D$, and $I = D$. When $I = D$, NMF trivially resolves to the natural latent space basis, i.e. the neuron directions. When studying EfficientNet we disregard NMF, since this network uses the SiLU activation function (Ramachandran et al., 2017) which allows negative feature activations, rendering NMF non-applicable. Tables 3,4, 5, 6, 7 summarize the comparative analysis for ResNet18, EfficientNet, Inception-v3, VGG16 and ResNet50, respectively. In the following subsections, we make a detailed discussion on those tables.

7.5.1 Analysis for ResNet18 trained on Places365

Clustering Quality: Regarding dataset coverage, both our EDDP variants explain 86% of the dataset regardless of cluster count. Specifically, this means that 86% of the patch embeddings in the concept dataset have been assigned to at least one cluster. This number is substantially higher than the coverage of the clustering obtained via NMF (which is at most 57%) or the natural latent space basis (49%) and still significantly higher than the coverage of the clustering obtained via PCA (at most 77%). As far as redundancy is concerned, the EDDP variants minimize multiple cluster assignments to individual patches, as they attain the lowest redundancy scores (at most 1.33 cluster assignments per patch). While NMF and the natural basis rank 3rd in redundancy terms with more than 1.77 assignments per patch, PCA is ranked last with the same number exceeding 7.27.

Interpretability: In classification metrics, the clustering of EDDP-U is the most interpretable of all, scoring higher than alternative clusterings, especially in Precision and AP terms. In most cases, clustering with

Table 3: Comparative Analysis of our Encoding-Decoding Direction Pairs (EDDP) against the Unsupervised State-of-the-Art. This table summarizes metrics for ResNet18 trained on Places365. EDDP-U stands for using Unconstrained Feature Manipulation and EDDP-C for using Constrained Feature Manipulation.

				ResNet18 / Places365								
I	Method	Coverage ↑	Redundancy ↓	Precision ↑	Recall ↑	F1 ↑	AP ↑	$\mathcal{M}$ ↓	$\mathcal{S}^1$ ↑	$\mathcal{S}^2$ ↑	mIoU ↑	$\mathcal{I}^1$ ↑
384	PCA	0.72	7.27	0.26±0.13	0.14±0.11	0.18±0.11	0.17±0.11	7.47	16.57	5.6	0.04	**0.73**
	NMF	0.57	2.06	0.62±0.19	0.21±0.14	0.31±0.17	0.4±0.18	6.88	29.56	17.43	0.08	0.68
	EDDP-U	**0.86**	**1.29**	**0.82±0.21**	**0.23±0.16**	**0.33±0.18**	**0.53±0.19**	**6.61**	**41.73**	**28.01**	**0.12**	0.58
	EDDP-C	**0.86**	1.32	0.81±0.21	**0.23±0.16**	**0.33±0.17**	0.5±0.19	6.67	41.5	27.49	**0.12**	0.61
448	PCA	0.75	8.89	0.25±0.12	0.14±0.11	0.17±0.11	0.16±0.1	7.48	18.06	5.62	0.04	**0.73**
	NMF	0.51	1.79	0.67±0.18	0.21±0.14	0.31±0.17	0.43±0.18	6.96	31.77	18.16	0.07	0.69
	EDDP-U	**0.86**	**1.32**	**0.83±0.19**	**0.22±0.16**	**0.32±0.18**	**0.53±0.19**	**6.64**	**47.5**	**32.07**	**0.11**	0.59
	EDDP-C	**0.86**	1.33	0.82±0.2	0.21±0.16	0.31±0.18	0.49±0.19	6.72	46.3	31.34	**0.11**	0.61
512	Natural	0.49	1.79	0.69±0.18	0.2±0.13	0.3±0.16	0.43±0.17	7.02	34.61	18.74	0.07	0.69
	PCA	0.77	10.05	0.25±0.12	0.14±0.11	0.17±0.11	0.16±0.1	7.5	19.41	5.62	0.04	**0.74**
	EDDP-U	**0.86**	**1.28**	**0.82±0.22**	**0.21±0.17**	**0.31±0.19**	**0.51±0.21**	**6.66**	**52.51**	**37.78**	**0.11**	0.61
	EDDP-C	**0.86**	**1.28**	0.81±0.24	0.2±0.16	0.29±0.19	0.47±0.2	6.73	50.29	36.99	0.1	0.63

EDDP-C attains scores close to clustering with EDDP-U. Thus, EDDP-C is ranked 2nd in all classification metrics except in the case of F1 score and $I = 512$, in which the natural basis is slightly better by a score point of 0.01. With only the latter exception, in all classification metrics, NMF and the natural basis are ranked 3rd, while PCA is ranked last.

The high precision of our concept detectors (approximately 0.82 on average) indicates that the learned directions are highly monosemantic. The latter is additionally confirmed by the monosemanticity metric based on CLIP embedding distances, in which EDDP variants are attributed the lowest $\mathcal{M}$ score. Comparing with the rest of the approaches, all of the clusterings obtained by NMF, the natural basis, and PCA are less monosemantic, often by a large margin (0.67 precision for NMF, 0.26 precision for PCA and 0.69 for the natural basis).

Similar conclusions can be drawn from the segmentation metrics, in which the concept detectors of EDDP score substantially higher than the previous approaches. For example, when $I = 448$, EDDP-C achieves 46.3 score points in $\mathcal{S}^1$, surpassing NMF's 31.77, and reaches 0.11 mIoU points in contrast to NMF's 0.07. Finally, the EDDP variants also achieve the most diverse clustering, covering a variety of visual concepts, as justified by the substantially higher values of $\mathcal{S}^2$ compared to the rest of the approaches. Furthermore, this diversity is consistently improved with the increase in cluster count, a phenomenon that is less prominent for the rest of the state-of-the-art baselines.

Influence: To rank the methods based on the network's sensitivity to the identified concepts (metric $\mathcal{I}^1$), starting from the most influential clustering, we would list PCA first, then NMF, followed by the Natural basis, and finally EDDP-C and EDDP-U. In this case, it appears that there is a clear anti-correlated relationship between interpretability and influence, with the most interpretable clustering being less influential on the overall model outcomes. We will be discussing this further at the end of the section.

7.5.2 Analysis for EfficientNet trained on ImageNet

Clustering Quality: Clusters created by the EDDP variants attain a Coverage score of 85%, while the best values for PCA and the natural basis in the same metric are 68% and 51%, respectively. In Redundancy terms, EDDP achieves scores less than 1.65, while the minimum scores for PCA and the natural basis are 19.29 and 5.44, respectively.

Interpretability: In terms of classification metrics, the directional clusterings obtained via EDDP-U and EDDP-C are approximately equally interpretable and notably more interpretable than the directional clustering of PCA. For instance, when $I = 1120$, the mean Precision of PCA's concept detectors is 0.28, the mean Recall 0.13, the mean F1 score 0.17, while the mean AP is equal to 0.19. For EDDP-U, the mean scores for the same metrics are 0.76 for Precision, 0.2 for Recall, 0.28 for F1 score, and 0.39 for AP. Similar conclusions about the improved interpretability of EDDP can be drawn when comparing with the natural latent space basis in the case of $I = 1280$.

Table 4: Comparative Analysis of our Encoding-Decoding Direction Pairs (EDDP) against the Unsupervised State-of-the-Art. This table summarizes metrics for EfficientNet (b0) trained on ImageNet. EDDP-U stands for using Unconstrained Feature Manipulation and EDDP-C for using Constrained Feature Manipulation.

				EfficientNet / ImageNet								
I	Method	Coverage ↑	Redundancy ↓	Precision ↑	Recall ↑	F1 ↑	AP ↑	$\mathcal{M}$ ↓	$\mathcal{S}^1$ ↑	$\mathcal{S}^2$ ↑	mIoU ↑	$\mathcal{I}^1$ ↑
960	PCA	0.63	19.29	0.29±0.08	0.13±0.07	0.18±0.07	0.19±0.07	7.44	**35.26**	2.62	**0.04**	**0.95**
	EDDP-U	**0.85**	1.51	**0.75±0.22**	**0.2±0.17**	**0.27±0.17**	**0.38±0.16**	**6.74**	27.92	**14.71**	0.03	0.94
	EDDP-C	**0.85**	**1.48**	0.72±0.23	**0.2±0.18**	**0.27±0.17**	**0.38±0.17**	6.75	25.92	14.45	0.03	0.94
1120	PCA	0.67	24.7	0.28±0.07	0.13±0.07	0.17±0.07	0.19±0.07	7.44	**42.33**	2.7	**0.04**	**0.95**
	EDDP-U	**0.85**	1.61	**0.76±0.21**	**0.2±0.17**	**0.28±0.17**	**0.39±0.17**	**6.73**	31.36	**16.54**	0.03	0.94
	EDDP-C	**0.85**	**1.54**	0.74±0.22	**0.2±0.18**	**0.28±0.19**	**0.39±0.17**	6.74	28.62	16.38	0.03	0.94
1280	Natural	0.51	5.44	0.56±0.13	0.14±0.07	0.21±0.1	0.29±0.12	7.35	35.94	7.09	0.03	**0.95**
	PCA	0.68	26.71	0.28±0.08	0.13±0.07	0.17±0.07	0.18±0.07	7.44	**48.01**	3.12	**0.04**	**0.95**
	EDDP-U	**0.85**	1.65	**0.74±0.21**	**0.19±0.16**	**0.27±0.16**	**0.36±0.17**	**6.81**	40.38	**19.12**	0.03	0.94
	EDDP-C	**0.85**	**1.6**	0.73±0.21	**0.19±0.17**	0.26±0.17	**0.36±0.17**	6.88	36.95	18.98	0.03	0.94

Regarding monosemanticity, the concept detectors of EDDP attain a mean Precision score which is better than 0.72, in contrast to the ones of PCA, which attain mean Precision scores below 0.29. The same gap between PCA and EDDP is similarly reflected in the $\mathcal{M}$ score. For example, when $I = 1120$, the $\mathcal{M}$ score of EDDP-C is 6.74 while the score of PCA is 7.44. EDDP also demonstrates a substantial improvement in monosemanticity compared to the natural basis. EDDP-C attains a mean Precision score of 0.73, while the score of the natural basis for the same metric is only 0.56. Additionally, EDDP-C attains 6.88 points in terms of $\mathcal{M}$, which is significantly lower than the 7.35 points of the natural basis.

In the context of segmentation, when $I = 1120$, PCA's concept detectors exhibit improved performance concerning $\mathcal{S}^1$, exceeding EDDP-U by roughly 12 points. In mIoU terms, PCA still scores higher (0.04), but EDDP follows closely (0.03). Yet, PCA exhibits a narrow diversity in the clustering, discovering substantially fewer concepts than EDDP, as reflected in $\mathcal{S}^2$ in which EDDP-U surpasses PCA by up to approximately 14 points. When considering the natural basis as an alternative directional clustering, EDDP scores better in terms of $\mathcal{S}^1$ and $\mathcal{S}^2$ and equally well in mIoU.

Influence: With respect to the impact of the learned directions on the network predictions, EfficientNet shows a significant sensitivity to the direction set determined by PCA or the neuron directions from the natural basis, with a $\mathcal{I}^1$ score of 0.95. Even though the model is less influenced by the directions learned with EDDP, this is only by a small margin, as the $\mathcal{I}^1$ scores for EDDP variants are 0.94.

7.5.3 Analysis for Inception-v3 trained on ImageNet

Table 5: Comparative Analysis of our Encoding-Decoding Direction Pairs (EDDP) against the Unsupervised State-of-the-Art. This table summarizes metrics for Inception-v3 trained on ImageNet. EDDP-U stands for using Unconstrained Feature Manipulation and EDDP-C for using Constrained Feature Manipulation.

				Inception-v3 / ImageNet								
I	Method	Coverage ↑	Redundancy ↓	Precision ↑	Recall ↑	F1 ↑	AP ↑	$\mathcal{M}$ ↓	$\mathcal{S}^1$ ↑	$\mathcal{S}^2$ ↑	mIoU ↑	$\mathcal{I}^1$ ↑
1536	PCA	0.7	32.29	0.26±0.12	0.12±0.1	0.16±0.1	0.17±0.1	7.39	54.5	4.19	0.04	**0.95**
	NMF	0.7	9.26	0.53±0.17	0.16±0.12	0.24±0.14	0.28±0.16	7.24	70.68	14.92	0.05	**0.95**
	EDDP-U	**0.87**	2.41	0.84±0.18	**0.28±0.24**	**0.38±0.26**	0.53±0.26	**6.79**	**156.46**	**28.03**	**0.11**	0.93
	EDDP-C	0.85	**1.9**	**0.86±0.19**	0.23±0.16	0.33±0.19	**0.58±0.24**	6.87	125.64	27.46	0.08	0.94
1792	PCA	0.68	33.26	0.28±0.12	0.12±0.1	0.17±0.1	0.17±0.1	7.39	59.18	4.1	0.03	**0.95**
	NMF	0.64	7.71	0.6±0.18	0.16±0.13	0.25±0.16	0.32±0.17	7.29	72.86	15.86	0.04	**0.95**
	EDDP-U	**0.9**	2.96	0.86±0.16	**0.33±0.25**	**0.43±0.26**	0.58±0.25	**6.77**	**210.44**	**25.77**	**0.13**	0.93
	EDDP-C	0.86	**2.19**	**0.89±0.16**	0.24±0.16	0.36±0.19	**0.62±0.21**	6.92	174.0	24.69	0.1	0.94
2048	Natural	0.63	10.29	0.58±0.17	0.17±0.13	0.25±0.15	0.31±0.17	7.35	84.62	14.27	0.04	**0.95**
	PCA	0.71	42.35	0.26±0.12	0.12±0.1	0.16±0.1	0.17±0.1	7.38	69.87	4.24	0.03	**0.95**
	EDDP-U	0.86	**2.36**	**0.85±0.2**	**0.31±0.29**	**0.4±0.29**	**0.54±0.28**	**6.95**	**170.81**	**32.13**	**0.09**	0.94
	EDDP-C	**0.93**	3.98	0.75±0.18	0.16±0.12	0.24±0.14	0.38±0.16	7.09	92.67	31.18	0.05	0.94

Clustering Quality: On par with the experiments on the previous architectures, EDDP variants explain more than the 85% of the concept dataset, as noted by the respective Coverage scores. This score is still significantly higher than the ones attained from NMF (up to 70%), the natural basis (63%) or PCA (up to 71%). As far as Redundancy is concerned, on one hand, EDDP does not exceed 3.98 cluster assignments per patch. On the other hand, NMF assigns a patch to more than 7.71 clusters, while for PCA this number exceeds 32.29. Finally, in the clustering obtained by the use of the natural basis, each patch is assigned to 10.29 clusters.

Interpretability: For $I = 1536$ and $I = 1792$, the concept detectors of the EDDP variants score substantially higher in the classification metrics than the rest of the approaches. For example, when $I = 1792$, EDDP-C attains a Precision score of 0.89, whereas the same score for NMF is 0.6 and for PCA 0.28. For the same I, EDDP-U attains an F1 score of 0.43, which is a notable improvement over NMF's 0.25 and PCA's 0.17. Finally, in terms of AP, EDDP-C achieves a score of 0.62 points, which is significantly more competitive than the score of NMF (0.32) and PCA (0.17). For $I = 2048$, concept detectors from EDDP-U consistently score higher in the classification metrics than any other approach. Unlike what we have seen in the rest of the experiments, in that case, EDDP-C did not follow EDDP-U closely in the classification metrics. Instead, it is clearly ranked 2nd, surpassing PCA and the natural basis in Precision and AP while remaining comparable with the natural basis in Recall and F1 score.

Regarding monosemanticity, EDDP-U attains Precision scores close to 0.84, while for the cases of $I = 1536$ and $I = 1792$, EDDP-C exceeds this number, achieving scores up to 0.89 but attains a lower score of 0.75 when $I = 2048$. The best Precision score for NMF is 0.6 for $I = 1792$, while for PCA this score is 0.28. Finally, when clustering with the directions of the neurons, i.e. the natural basis, the Precision score is 0.58. When measuring monosemanticity with the CLIP embedding distances, the EDDP variants achieve a substantially lower score compared to the rest of the approaches. For instance, when $I = 1792$, the EDDP-U clustering attains a score of 6.77, EDDP-C 6.92, NMF 7.29 and PCA 7.39. Interestingly, unlike what we have seen when using the labeled dataset in terms of Precision, when $I = 2048$ EDDP-C and EDDP-U score similarly in $\mathcal{M}$, with EDDP-U attaining a score of 6.95 and EDDP-C 7.09.

As far as segmentation is concerned, the ranking of the methods is consistent across all metrics: EDDP-U comes first, followed by EDDP-C, then NMF or the natural basis, and finally PCA. Beyond just ranking, the gap in the scores between EDDP and other approaches is large. For instance, when $I = 1536$, the EDDP-U score in terms of $\mathcal{S}^1$ is 156.46 when NMF's is 70.68. Similarly, for the same case, EDDP-U's $\mathcal{S}^2$ is 28.03 when NMF's is 14.92, while for mIoU, EDDP-U's score is 0.11 when NMF's is 0.05.

Influence: Regarding the sensitivity of the model with respect to the identified concepts, Inception-v3 is more sensitive to the PCA and NMF directions with a $\mathcal{I}^1$ score of 0.95. The network is slightly less sensitive to the concepts identified by EDDP-C and EDDP-U, but once again by a small margin. EDDP-C attains a $\mathcal{I}^1$ score of 0.94 and EDDP-U a score in $\{0.93, 0.94\}$.

7.5.4 Analysis for VGG16 trained on ImageNet

Table 6: Comparative Analysis of our Encoding-Decoding Direction Pairs (EDDP) against the Unsupervised State-of-the-Art. This table summarizes metrics for VGG16 trained on ImageNet. EDDP-U stands for using Unconstrained Feature Manipulation and EDDP-C for using Constrained Feature Manipulation.

				VGG16 / ImageNet								
I	Method	Coverage ↑	Redundancy ↓	Precision ↑	Recall ↑	F1 ↑	AP ↑	$\mathcal{M}$ ↓	$\mathcal{S}^1$ ↑	$\mathcal{S}^2$ ↑	mIoU ↑	$\mathcal{I}^1$ ↑
384	PCA	0.64	7.31	0.29±0.09	0.15±0.07	0.19±0.07	0.16±0.07	7.85	22.44	2.98	0.06	0.87
	NMF	0.55	1.6	0.6±0.16	0.17±0.11	0.26±0.13	**0.31±0.14**	7.44	22.73	**9.7**	0.06	0.87
	EDDP-U	**0.82**	1.17	0.61±0.18	**0.18±0.09**	**0.27±0.09**	**0.31±0.12**	**6.88**	**29.98**	9.39	**0.08**	**0.91**
	EDDP-C	0.79	**1.07**	**0.63±0.18**	0.16±0.09	0.24±0.09	**0.31±0.12**	6.92	26.23	8.89	0.07	0.9
448	PCA	0.67	8.91	0.28±0.08	0.15±0.07	0.19±0.07	0.16±0.06	7.86	25.8	3.12	0.06	0.87
	NMF	0.5	1.44	**0.62±0.16**	0.16±0.1	0.25±0.12	**0.31±0.14**	7.44	24.82	9.86	0.06	0.87
	EDDP-U	**0.84**	1.35	0.59±0.18	**0.18±0.09**	**0.26±0.09**	0.3±0.11	**6.93**	**34.67**	**10.29**	**0.08**	**0.91**
	EDDP-C	0.82	**1.22**	0.61±0.18	0.16±0.08	0.24±0.09	0.3±0.11	**6.93**	30.91	9.26	0.07	0.9
512	Natural	0.58	2.12	0.58±0.16	0.16±0.1	0.25±0.12	0.29±0.12	7.5	30.61	10.28	0.06	0.87
	PCA	0.69	9.62	0.29±0.08	0.15±0.06	0.19±0.07	0.16±0.06	7.87	30.25	3.51	0.06	0.86
	EDDP-U	**0.85**	1.43	0.61±0.18	**0.18±0.08**	**0.27±0.09**	**0.31±0.11**	**6.95**	**41.2**	**11.11**	**0.08**	**0.91**
	EDDP-C	**0.85**	**1.37**	**0.62±0.18**	0.15±0.09	0.24±0.09	0.3±0.11	7.09	33.91	10.83	0.07	0.9

Clustering Quality: In terms of clustering quality metrics, the EDDP variants attain higher Coverage and lower Redundancy scores than either one of NMF, PCA, or the natural basis, in a similar fashion as in the rest of the architectures.

Interpretability: Unlike the rest of the architectures, in classification metrics, NMF and the EDDP variants perform on par. For example, when $I = 448$, NMF attains a Precision score of 0.62 exceeding EDDP-U's 0.59. In Recall and F1 score terms, EDDP-U achieves the highest scores of 0.18 and 0.26, respectively, while for NMF these numbers are 0.16 and 0.25. In terms of AP, NMF scores 0.31 while both EDDP variants attain a score of 0.30. In most cases, all of NMF, the natural basis, and EDDP substantially surpass the clustering of PCA in the classification metrics.

Even though EDDP, NMF and the natural latent space basis score similarly in Precision terms, when monosemanticity is measured via the CLIP embedding distances, the EDDP variants achieve the best scores, often by a substantial margin. For instance, when $I = 384$, NMF achieves an $\mathcal{M}$ score of 7.44, PCA a score of 7.85, while EDDP-U a score of 6.88.

Finally, in segmentation metrics, EDDP variants achieve the highest scores in $\mathcal{S}^1$ and mIoU, while in $\mathcal{S}^2$, EDDP-U is ranked 1st in two of the three cases ($I = 448$ and $I = 512$) while ranked 2nd, after NMF in the third case ($I = 384$).

Influence: Regarding the sensitivity of VGG16 with respect to the concepts, the network is the most sensitive towards the directions learned with EDDP-U ($\mathcal{I}^1$ score of 0.91), followed by EDDP-C ($\mathcal{I}^1$ score of 0.9) and last, by NMF, the natural basis, or PCA with $\mathcal{I}^1$ scores close to 0.87.

7.5.5 Analysis for ResNet50 trained on Moments in Time

Table 7: Comparative Analysis of our Encoding-Decoding Direction Pairs (EDDP) against the Unsupervised State-of-the-Art. This table summarizes metrics for ResNet50 trained on Moments in Time (MiT). EDDP-U stands for using Unconstrained Feature Manipulation and EDDP-C for using Constrained Feature Manipulation.

				ResNet50 / MiT								
I	Method	Coverage ↑	Redundancy ↓	Precision ↑	Recall ↑	F1 ↑	AP ↑	$\mathcal{M}$ ↓	$\mathcal{S}^1$ ↑	$\mathcal{S}^2$ ↑	mIoU ↑	$\mathcal{I}^1$ ↑
1536	PCA	0.7	30.77	0.16±0.06	0.1±0.05	0.12±0.05	0.1±0.04	7.34	58.51	3.55	0.04	**0.88**
	NMF	0.54	9.07	0.46±0.17	0.16±0.11	0.23±0.13	0.27±0.13	6.91	73.38	17.31	0.05	0.85
	EDDP-U	0.84	**2.13**	0.72±0.22	**0.17±0.12**	**0.26±0.15**	0.36±0.16	**6.25**	**127.83**	33.67	**0.08**	0.85
	EDDP-C	**0.88**	2.37	**0.75±0.19**	**0.17±0.11**	**0.26±0.13**	**0.45±0.14**	6.49	98.52	**34.81**	0.06	0.84
1792	PCA	0.72	36.06	0.16±0.06	0.1±0.05	0.12±0.05	0.1±0.04	7.35	65.82	3.58	0.04	**0.88**
	NMF	0.42	6.02	0.57±0.15	0.15±0.08	0.23±0.1	0.3±0.11	6.95	77.02	19.0	0.04	0.85
	EDDP-U	0.85	**2.47**	**0.78±0.16**	**0.19±0.1**	**0.29±0.13**	0.4±0.14	**6.24**	**162.86**	34.17	**0.09**	0.85
	EDDP-C	**0.88**	2.62	0.76±0.16	0.16±0.11	0.25±0.13	**0.44±0.13**	6.5	113.9	**36.68**	0.06	0.84
2048	Natural	0.5	11.18	0.47±0.16	0.15±0.09	0.22±0.11	0.26±0.12	6.97	90.35	16.63	0.04	0.85
	PCA	0.76	43.2	0.15±0.06	0.1±0.05	0.12±0.05	0.1±0.04	7.35	74.3	3.61	0.04	**0.88**
	EDDP-U	0.86	3.15	**0.72±0.2**	**0.21±0.13**	**0.31±0.16**	**0.43±0.16**	**6.29**	**209.2**	33.04	**0.1**	0.85
	EDDP-C	**0.88**	**2.83**	**0.72±0.16**	0.15±0.11	0.24±0.12	**0.43±0.13**	6.61	126.46	**35.98**	0.06	0.84

Clustering Quality: Once again, in clustering quality terms, the EDDP variants demonstrate both larger Coverage and lower Redundancy compared to the rest of the approaches, often with a large margin. When $I = 1792$, the coverage score for EDDP-C is 0.88 while for NMF it is 0.42. The gap between the two is more than twice the score of NMF. Similarly, the redundancy score of EDDP-C is 2.62 whereas NMF's is 6.02, with a similar conclusion regarding the gap between the two.

Interpretability: The clustering obtained via EDDP is more interpretable in terms of classification metrics, especially in Precision, AP, and sometimes in the F1 score as well. Regardless of whether monosemanticity is measured via Precision or distances between CLIP embeddings, the EDDP variants score better, similar to the rest of the experiments.

When considering segmentation, both EDDP variants demonstrate consistent superiority in terms of $\mathcal{S}^1$ and $\mathcal{S}^2$ and mIoU. Interestingly, in this experiment, EDDP-C scores the highest in $\mathcal{S}^2$, indicating a clustering that captures a larger variety of concepts.

Influence: In terms of the concept sensitivity metric $\mathcal{I}^1$, NMF, EDDP-C, EDDP-U and the natural basis perform on par, with an approximate score of 0.85. On the contrary, PCA achieves a score of 0.88, which brings it further ahead of the competition.

7.5.6 Discussion

From the previous experiments, we can draw the following, mostly straightforward, conclusions: a) EDDP's directional clusters are monosemantic, often surpassing the previous state-of-the-art by a significant margin in monosemanticity metrics. b) EDDP also excels in terms of F1 score, where EDDP-U is consistently ranked first among the competition, and EDDP-C is often ranked second. c) In terms of segmentation and specifically $\mathcal{S}^1$, EDDP-U is consistently ranked first, except for EfficientNet in which the clustering of PCA scores better, yet with substantially inferior performance in most of the other interpretability metrics. In the same metric, EDDP-C is often ranked second. d) In terms of discovering a diverse set of concepts ($\mathcal{S}^2$) the EDDP variants score the best, often by a large margin, except for one case in VGG16 where they score on par with the best method. e) In terms of influence, in all cases except VGG16, the EDDP variants are ranked last. However, in many cases, the respective score is not far behind the competition.

In most cases, and in a broader sense, we observe that interpretability is somewhat negatively correlated with influence. Less interpretable directions may represent complex interactions (i.e. correspond to less pure human-understandable concepts) and, as a result, they are more impactful on the network predictions, in the sense that they affect many output classes. On the contrary, more interpretable directions may have a more targeted impact on specific output classes, and thus score lower in the respective metric.

7.6 Ablation Study

7.6.1 Interpretability Losses

Table 8: Ablation study with respect to the interpretability losses. For ResNet18 $I = 448$, and for EfficientNet $I = 1120$.

Ortho	$\mathcal{L}^{fs}$	$\mathcal{L}^{eac}$	Coverage ↑	Redundancy ↓	Precision ↑	Recall ↑	F1 ↑	AP ↑	$\mathcal{M}$ ↓	$\mathcal{S}^1$ ↑	$\mathcal{S}^2$ ↑	mIoU ↑
						ResNet18 / Places365						
✓	✗	✗	**0.89**	2.25	0.71±0.19	**0.3±0.18**	**0.4±0.19**	0.47±0.19	**6.44**	**54.28**	26.4	**0.13**
✗	✗	✗	0.86	**1.09**	**0.88±0.17**	0.18±0.12	0.29±0.15	**0.54±0.17**	6.57	40.92	19.1	0.1
✗	✓	✗	0.83	1.13	0.85±0.19	0.19±0.14	0.29±0.16	0.53±0.18	6.57	39.26	25.36	0.1
✗	✓	✓	0.85	1.29	0.83±0.19	0.22±0.15	0.31±0.17	0.52±0.18	6.64	47.14	**29.0**	0.11
						EfficientNet / ImageNet						
✓	✗	✗	**0.9**	3.36	0.67±0.19	0.17±0.14	0.25±0.14	0.34±0.14	7.0	**46.9**	14.42	**0.04**
✗	✗	✗	0.84	**1.29**	**0.78±0.23**	**0.23±0.21**	**0.3±0.2**	0.39±0.18	6.81	19.54	13.29	0.02
✗	✓	✗	**0.86**	1.59	**0.78±0.2**	0.2±0.16	0.29±0.16	**0.4±0.17**	**6.68**	25.42	14.1	0.03
✗	✓	✓	0.85	1.57	0.74±0.2	0.22±0.18	**0.3±0.17**	0.38±0.17	**6.68**	28.72	**16.02**	0.03

As already discussed previously, the motivation behind the loss terms that we introduced in Section 4.2 is to sustain or improve the interpretability of the clustering when moving from an orthogonal decoding direction set to a non-orthogonal one. In Table 8 we present interpretability metrics for the cases when we learn the directions with $\mathcal{L}^{fs}$, both $\mathcal{L}^{fs}$ and $\mathcal{L}^{eac}$, or without any of them. We also provide metrics for the case of orthogonal decoding directions (marked as *Ortho*). The latter is equivalent to learning with the method of Doumanoglou et al. (2023) using the Augmented Lagrangian loss of Section 4.5. We provide results regarding the directions learned for ResNet18 and EfficientNet. In these experiments, we exclude any form of Uncertainty Region Alignment.

In both network case studies, starting without our interpretability losses and gradually adding them one after the other, we observe that the different variations a) compare similarly in coverage and redundancy terms and b) achieve comparable performance in classification and monosemanticity metrics. However, the impact of the loss terms on the segmentation metrics is more significant, especially in terms of $\mathcal{S}^1$ and $\mathcal{S}^2$. We emphasize the improvement in $\mathcal{S}^2$ since this metric captures the variety of the identified concepts. Compared to the orthogonal direction set, directions learned without orthogonality constraints a) result in a less redundant clustering, b) the monosemanticity of the clustering in terms of Precision is improved, and c) the clustering becomes more diverse, capturing a variety of different concepts.

Table 9: Ablation study with respect to the Unconstrained Uncertainty Region Alignment loss. For ResNet18 $I = 448$, for EfficientNet $I = 1120$, and for ResNet50 $I = 1792$.

Ortho	$\mathcal{L}^{uur}$	Coverage ↑	Redundancy ↓	Precision ↑	Recall ↑	F1 ↑	AP ↑	$\mathcal{M}$ ↓	$\mathcal{S}^1$ ↑	$\mathcal{S}^2$ ↑	mIoU ↑
				ResNet18 / Places365							
✓	✗	**0.89**	2.25	**0.71±0.19**	0.3±0.18	0.4±0.19	0.47±0.19	**6.44**	54.28	**26.4**	**0.13**
✓	✓	0.88	**2.2**	**0.71±0.18**	**0.31±0.18**	**0.41±0.19**	**0.48±0.19**	6.52	**54.56**	26.06	**0.13**
✗	✗	0.85	**1.29**	**0.83±0.19**	**0.22±0.15**	0.31±0.17	0.52±0.18	**6.64**	47.14	29.0	**0.11**
✗	✓	**0.86**	1.32	**0.83±0.19**	**0.22±0.16**	**0.32±0.18**	**0.53±0.19**	**6.64**	**47.5**	**32.07**	**0.11**
				EfficientNet / ImageNet							
✓	✗	**0.9**	3.36	0.67±0.19	**0.17±0.14**	**0.25±0.14**	0.34±0.14	7.0	46.9	14.42	0.04
✓	✓	**0.9**	**3.34**	**0.68±0.2**	**0.17±0.14**	**0.25±0.14**	**0.36±0.15**	**6.98**	**52.94**	**16.38**	**0.05**
✗	✗	**0.85**	**1.57**	0.74±0.2	**0.22±0.18**	**0.3±0.17**	0.38±0.17	**6.68**	28.72	16.02	**0.03**
✗	✓	**0.85**	1.61	**0.76±0.21**	0.2±0.17	0.28±0.17	**0.39±0.17**	6.73	**31.36**	**16.54**	**0.03**
				ResNet50 / MiT							
✓	✗	**0.88**	3.44	0.72±0.15	0.16±0.1	0.25±0.13	0.35±0.14	**6.47**	121.67	29.41	0.07
✓	✓	**0.88**	**3.31**	**0.73±0.16**	**0.18±0.1**	**0.27±0.13**	**0.37±0.13**	6.49	**137.76**	**33.0**	**0.08**
✗	✗	0.83	**2.42**	0.75±0.19	0.15±0.12	0.24±0.15	0.32±0.14	**6.1**	157.54	30.81	0.09
✗	✓	**0.85**	2.47	**0.78±0.16**	**0.19±0.1**	**0.29±0.13**	**0.4±0.14**	6.24	**162.86**	**34.17**	**0.09**

Table 10: Ablation study with respect to the Uncertainty Region Alignment losses. For ResNet18 $I = 448$, for EfficientNet $I = 1120$, and for ResNet50 $I = 1792$.

$\mathcal{L}^{uur}$	$\mathcal{L}^{cur}$	Coverage ↑	Redundancy ↓	Precision ↑	Recall ↑	F1 ↑	AP ↑	$\mathcal{M}$ ↓	$\mathcal{S}^1$ ↑	$\mathcal{S}^2$ ↑	mIoU ↑	SDC ↑	SCDP ↑
					ResNet18 / Places365								
✗	✗	0.85	**1.29**	**0.83±0.19**	**0.22±0.15**	0.31±0.17	0.52±0.18	**6.64**	47.14	29.0	**0.11**	291	**2104**
✓	✗	**0.86**	1.32	**0.83±0.19**	**0.22±0.16**	**0.32±0.18**	**0.53±0.19**	**6.64**	**47.5**	**32.07**	**0.11**	264	1565
✗	✓	**0.86**	1.33	0.82±0.2	0.21±0.16	0.31±0.18	0.49±0.19	6.72	46.3	31.34	**0.11**	**304**	1692
					EfficientNet / ImageNet								
✗	✗	**0.85**	1.57	0.74±0.2	**0.22±0.18**	**0.3±0.17**	0.38±0.17	**6.68**	28.72	16.02	**0.03**	93	216
✓	✗	**0.85**	1.61	**0.76±0.21**	0.2±0.17	0.28±0.17	**0.39±0.17**	6.73	**31.36**	**16.54**	**0.03**	107	243
✗	✓	**0.85**	**1.54**	0.74±0.22	0.2±0.18	0.28±0.19	**0.39±0.17**	6.74	28.62	16.38	**0.03**	**673**	**1484**
					ResNet50 / MiT								
✗	✗	0.83	**2.42**	0.75±0.19	0.15±0.12	0.24±0.15	0.32±0.14	**6.1**	157.54	30.81	**0.09**	370	548
✓	✗	0.85	2.47	**0.78±0.16**	**0.19±0.1**	**0.29±0.13**	0.4±0.14	6.24	**162.86**	34.17	**0.09**	393	570
✗	✓	**0.88**	2.62	0.76±0.16	0.16±0.11	0.25±0.13	**0.44±0.13**	6.5	113.9	**36.68**	0.06	**1353**	**3913**

7.6.2 Uncertainty Region Alignment

In this section we study how Uncertainty Region Alignment may affect the interpretability of the clustering and the discovery of concepts with significant influence on the network predictions. For this study we consider three network architectures: ResNet18, EfficientNet, and ResNet50 trained on the datasets already discussed in Section 7.1.

In Table 9 we compare, in quality and interpretability terms, the clusterings obtained with and without the Unconstrained Uncertainty Region Alignment loss ($\mathcal{L}^{uur}$). We consider learning the decoding directions both with and without orthogonality constraints (*Ortho*). Some simple conclusions that can be drawn from the experiments are: a) Coverage may be improved when using it but Redundancy can be slightly worsened, b) the Precision and AP of the concept detectors are consistently improved by its use, c) it consistently improves the performance of concept detectors in terms of $\mathcal{S}^1$, and d) $\mathcal{L}^{uur}$ can significantly improve the variety of concepts captured by the direction set ($\mathcal{S}^2$ metric).

In Table 10 we focus on comparing between the two Uncertainty Region Alignment variants by additionally considering metrics of concept influence. For the latter, we use RCAV's statistical significance test in which we ground our SDC and SCDP metrics (Section 7.1). Some key takeaways drawn from these experiments for using $\mathcal{L}^{cur}$ are: a) Coverage may be improved by its use, but Redundancy can be a bit worsened, b) the concept detectors' interpretability in terms of classification metrics is slightly inferior but somewhat comparable to when using $\mathcal{L}^{uur}$, c) in two of the three cases (ResNet18 and EfficientNet) the segmentation metrics across Uncertainty Region Alignment variants are mostly comparable, but in the third case (ResNet50) $\mathcal{L}^{cur}$ leads to a more diverse clustering (improved $\mathcal{S}^2$) but at the cost of a lower $\mathcal{S}^1$ score. d) In all cases, when comparing the two uncertainty region variants, the influence metrics favor $\mathcal{L}^{cur}$. In two of the three cases (EfficientNet and ResNet50) this improvement is substantially higher than what can be achieved when using $\mathcal{L}^{uur}$. For a more complete picture regarding the effect of $\mathcal{L}^{fso}$, which is used in EDDP-C but not in EDDP-U, see also Section A.10.

Overall, by this ablation study, we could conclude that the use of $\mathcal{L}^{uur}$ can improve the diversity of the clustering by capturing a larger variety of concepts, compared to when not using it. Using $\mathcal{L}^{cur}$ instead of $\mathcal{L}^{uur}$ may perform on par or improve this diversity, while substantially increasing the influence of the learned signal vectors on the network predictions, in a statistically significant sense.

7.7 Insights on Interpretability and Influence in comparison to Supervised Direction Learning

In this section, we compare our method with supervised direction learning, aiming to draw insights regarding interpretability and influence of concept directions. For this reason, we experiment with the last convolutional layer of ResNet18 trained on Places365. We consider our method with the constrained feature manipulation strategy, and two supervised learning approaches: a) IBD (Zhou et al., 2018) for supervised learning of decoding directions (i.e. concept detectors) and b) Pattern-CAVs (PCAVs) (Pahde et al., 2024) for supervised estimation of concept encoding directions. The supervised concept detectors and PCAVs are learned for the labels assigned to EDDP's concept detectors at the direction labeling phase (Section 3.4).

Interpretability: In the interpretability analysis, we consider three variants for the proposed method: a) the exact outcome of our method, marked as *EDDP*, b) combining directions with a shared label (post initial learning) using a binary linear classification layer which classifies representations positively if any detector with the same label does (marked as *EDDP - Linear OR*), and c) considering the learned directions but optimizing the classification threshold in a supervised manner, in a post-learning step, to enhance the F1 Score (marked as *EDDP /w sup thres*). This last approach assesses direction alignment to the concept by relaxing the sparsity constraint of the method. Table 11 summarizes metrics for this comparison. Results show that the classifiers of the proposed method achieve high Precision, comparable to the supervised ones, but suffer from low recall. The latter could be related to the strict sparsity objective of EDDP, as IBD exhibits significantly higher Redundancy. Combining classifiers with the same label improves recall, which indicates that different detectors capture different parts of the dataset, while supervised optimization of the classification bias further enhances F1 scores by relaxing sparsity.

Influence: In the concept influence analysis, we aim to answer whether PCAVs, that correspond to directions of high interpretability due to learning them with supervision, are more influential to the network predictions than signal vectors. Since Network Dissection can assign identical labels to multiple Encoding-Decoding Direction Pairs, direct comparison with Pattern-CAVs becomes less straightforward. We propose the following metric to help us draw some conclusions. Let $j \in \{0, 1, ..., N_l - 1\}$ index EDDP's signal vectors sharing the same concept label l, and $S^l_{j,k}$ represent the RCAV sensitivity score of the network relative to the j-th signal vector of label l when predicting class k. Similarly, let $S^l_{P,k}$ denote the sensitivity score of the network relative to the Pattern-CAV for the same label and class. Inspired by RCAV, we regard signal vectors as *noise vectors* and compare the sensitivity of the network with respect to PCAVs and signal vectors that share the same label. We define a metric $\mathcal{I}^2$, which when above 0.5 indicates that PCAVs have more influence than signal vectors on the network predictions at the statistical significance level of $\theta = 0.05$ with

Table 11: Comparison of EDDP (with CFM) with supervised direction learning Zhou et al. (2018). Comparing between: a) standard EDDP, b) combined concept detectors (*Linear-OR*) c) EDDP with the thresholds of concept detectors learned with supervision in a post initial direction learning step (*/w sup thres*), and d) IBD: a set of classifiers learned in a supervised way. The network here is ResNet18 and $I = 512$.

		ResNet18 / Places365							
Method	Coverage ↑	Redundancy ↓	Precision ↑	Recall ↑	F1 ↑	AP ↑	$\mathcal{S}^1$ ↑	$\mathcal{S}^2$ ↑	mIoU ↑
IBD Zhou et al. (2018)	0.95	3.08	0.84±0.13	0.6±0.17	0.68±0.15	0.77±0.15	54.71	54.71	0.2
EDDP	0.86	1.28	**0.81±0.24**	0.2±0.16	0.29±0.19	0.47±0.2	**50.29**	**36.99**	0.1
EDDP - Linear OR	N/A	N/A	0.73±0.25	0.35±0.26	0.4±0.22	**0.53±0.21**	30.77	30.77	**0.11**
EDDP - /w sup thres	N/A	N/A	0.6±0.19	**0.43±0.18**	**0.49±0.18**	0.47±0.2	N/A	N/A	N/A

Bonferroni correction:

$$\mathcal{I}^2 = \mathbb{E}_{l,k}\Big[\mathbb{1}(p_{l,k} < \frac{\theta}{N_l})\Big]$$

$$p_{l,k} = \frac{1}{N_l}\sum_j \mathbb{1}\big(|S^l_{j,k}| \geq |S^l_{P,k}|\big)$$

For RCAV $\alpha = 5.0$, $\mathcal{I}^2$ is equal to 0.34, which is less than 0.5 indicating the Pattern-CAVs are less influential on the network predictions than signal vectors. This outcome could also be linked to the discussion of Section 7.5.6. It looks like less interpretable directions (in that case EDDP's) have more influence on the network predictions compared to more interpretable ones.

7.8 Application: Global Model Explanations via Concept Sensitivity Testing

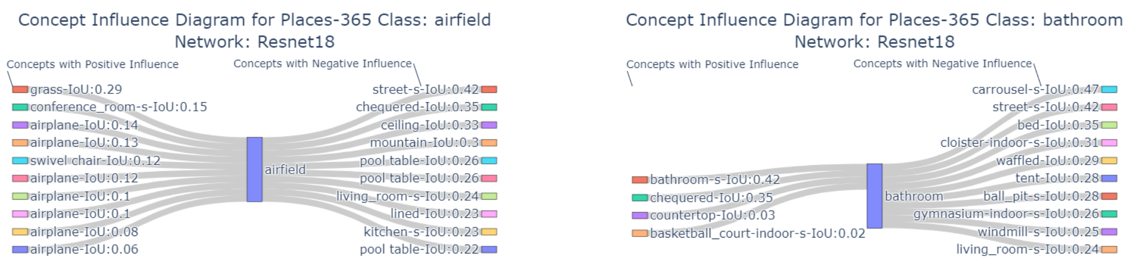

Figure 15: Concept Influence Diagram for ResNet18 trained on Places365. The model is sensitive to the depicted concepts with an absolute score above 0.99. (We use RCAV to quantify the sensitivity, and re-scale the score to $[-1, 1]$) Positive influencing and negative influencing concepts are provided. The number of concepts have been limited to 10. When concepts appear more than once, they correspond to different signal directions (as labeling the classifiers with NetDissect may assign the same concept name to more than one directions.) Here we report results for EDDP-C and $I = 512$.

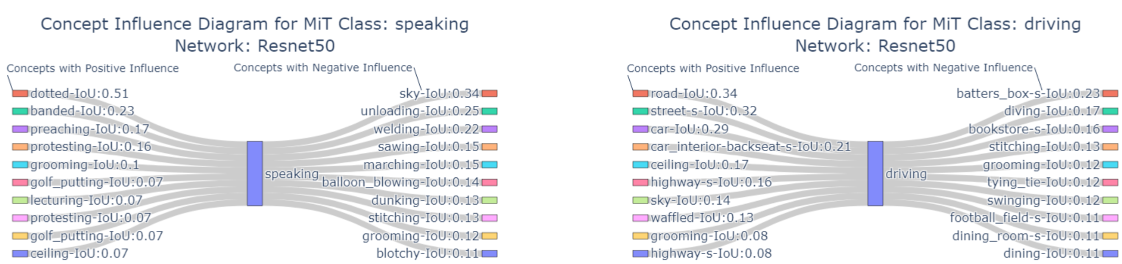

Figure 16: Concept Influence Diagram for ResNet50 trained on Moments in Time (MiT). The model is sensitive to the depicted concepts with an absolute score above 0.99. (We use RCAV to quantify the sensitivity, and re-scale the score to $[-1, 1]$) Positive influencing and negative influencing concepts are provided. The number of concepts have been limited to 10. When concepts appear more than once, they correspond to different signal directions (as labeling the classifiers with NetDissect may assign the same concept name to more than one directions.) Here we report results for EDDP-C and $I = 2048$.

Figures 15,40,41,42 depict concrete examples of how each concept's signal direction impacts the ResNet18's class predictions. Figures 16, 43 and 44 depict similar examples for ResNet50. Concepts appearing more than once correspond to different directions that have been attributed the same label by Network Dissection. Seemingly irrelevant concepts with positive influence may have three possible explanations: a) the network has some sensitivity to those concepts (as ResNet18's top1 accuracy is 56.51% and ResNet50's 28.4%) b)

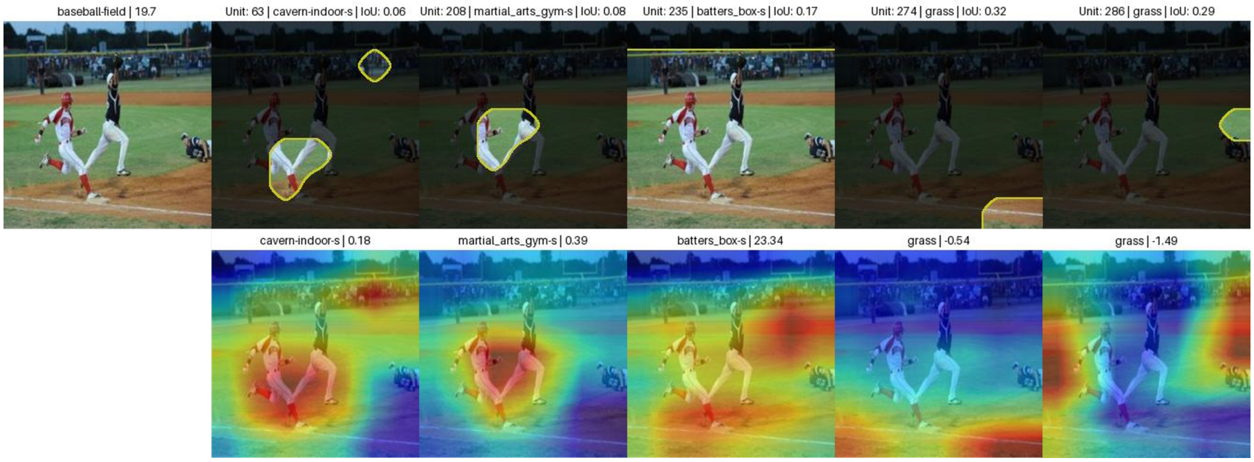

Figure 17: **Left:** Original image. The caption contains class prediction and output class logit. **Top Row:** Segmentation Maps obtained by the concept detectors. The caption contains classifier index (unit), concept-name and IoU score in the validation split of the dataset. **Bottom Row:** Concept Contribution Maps. The caption contains concept-name and contribution of the concept to the class logit.

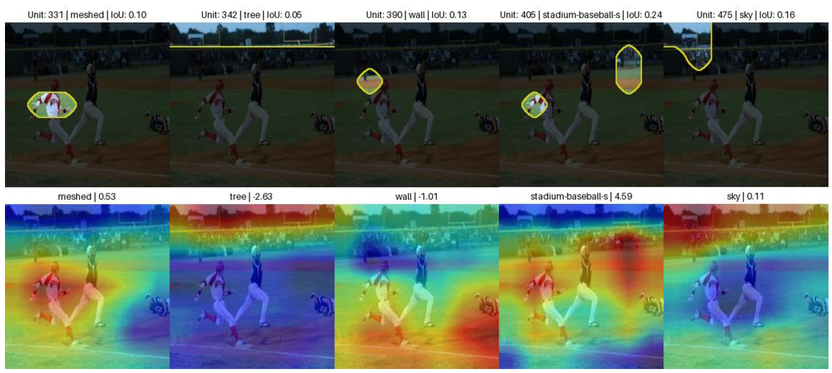

Figure 18: **Top Row:** Segmentation Maps obtained by the concept detectors. The caption contains classifier index (unit), concept-name and IoU score in the validation split of the dataset. **Bottom Row:** Concept Contribution Maps. The caption contains concept-name and contribution of the concept to the class logit.

their impact might be low, since RCAV only considers the sign of the class prediction difference before and after the perturbation, regardless of its magnitude, (thus those concepts may influence the prediction class positively, but by only a small amount) and c) their label may be misleading as the respective concept detectors do not reliably predict the concept (i.e. they exhibit a low IoU score).

7.9 Application: Local Model Explanations via Concept Contribution Maps

In this section, we apply the concept contribution analysis of Section 5.2 to provide a detailed local explanation for a prediction of ResNet18 in an image of Places365. In this example, we use direction pairs learned via EDDP-C and $I = 512$. The example input image (Fig. 17 top left) is correctly predicted to belong to the *baseball-field* class. The output class logit for this image is $l_c = 19.7$, the baseline logit is $l_b^m = 0.0003$ and the unexplainable residual of (27) is $r = 0.2816$. The top rows of Figures 17 and 18 provide segmentations which were obtained by applying our concept detectors to the patch embeddings of the input and subsequently upscaled to the original resolution. Each segmentation map highlights the region of the input that belongs to the detected concept. Above each segmentation map, we provide the index i of the respective concept detector (marked as *unit*), the name of the concept that was attributed to the concept detector by Network Dissection, and the dataset-wide Intersection over Union score of the detector when detecting the concept in the validation split of Broden. Below each segmentation map, we provide the respective Concept

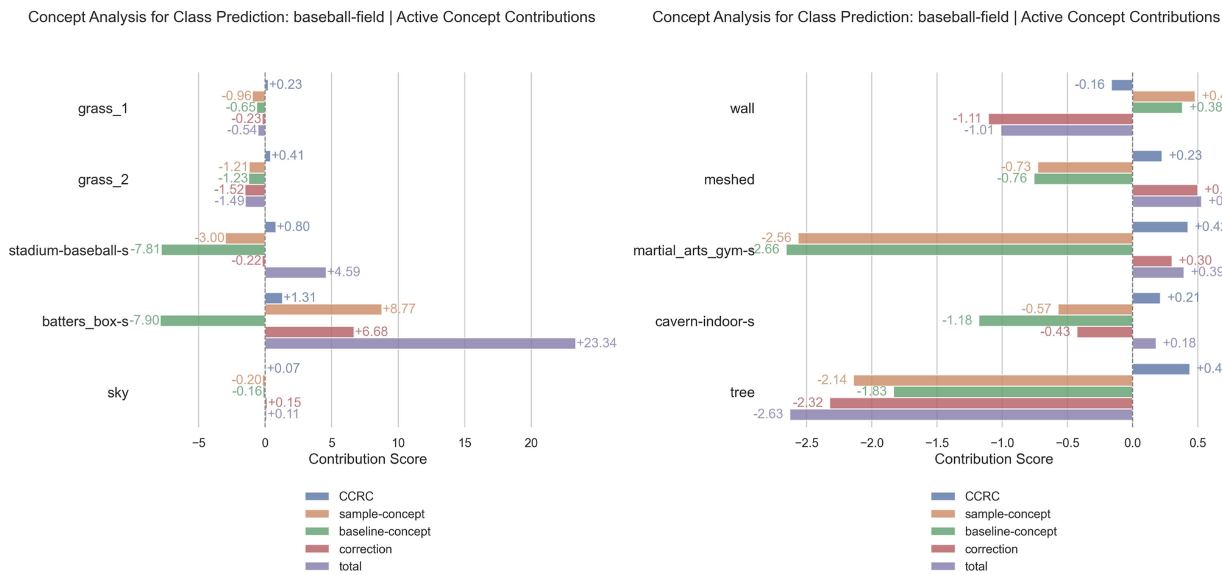

Figure 19: Concept Analysis for predicting an image of the *baseball-field* class. The figure depicts concepts found in the image. Even though concepts may share the same name, they correspond to different direction pairs.

Figure 20: Concept Analysis for predicting an image of the *baseball-field* class. The figure depicts top positive and top negative contributing concepts. Even though concepts may share the same name, they correspond to different direction pairs.

Contribution Map (CCM). Each spatial element $\boldsymbol{p}$ of CCM for concept i corresponds to the quantity $\phi^i_{\boldsymbol{p}}$ of (28). $\phi^i_{\boldsymbol{p}}$ contributes positively to the prediction in two cases: 1) whenever $\hat{v}_{\boldsymbol{p},i} - \hat{v}^b_{\boldsymbol{p},i} > 0$ (i.e. when the concept content in the sample is more than the concept content in the baseline point) and the Concept-Class Relation Coefficient (CCRC) $\boldsymbol{w}_c^T \hat{\boldsymbol{s}}_i$ is positive and 2) whenever $\hat{v}_{\boldsymbol{p},i} - \hat{v}^b_{\boldsymbol{p},i} < 0$, (i.e. when the concept content in the sample is less than the one in the baseline) and CCRC is negative. CCMs incorporate CCRC and thus they do not necessarily highlight the regions with the concept, as the sign of CCRC is integrated into the heatmaps (for instance: Unit 390). Above each CCM we provide the name of the concept together with the contribution of the CCM to the prediction logit after additionally integrating the correction factor of (27).

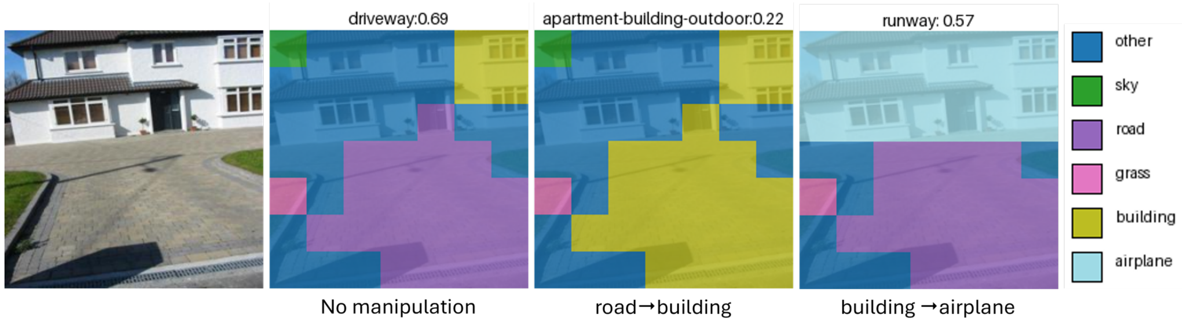

Figure 21: Counter-factual explanations via manipulating the patch embeddings in the representation space using directional concept arithmetic. **From Left to Right:** 1) original image, 2) segmentation map obtained by applying the learned concept detectors on the original image representation. The image is correctly predicted as *driveway* with confidence 69%. 3) Manipulate the latent representation and replace the *road* with the encoding of a *building*. Now the image is classified as *apartment-building-outdoor* with confidence 22%. 4) Manipulate the latent representation and replace the (whole) *building* with the encoding of an *airplane*. The manipulated image is classified as *runway* with confidence 57%.

Figures 19 and 20 depict image-level concept contributions by breaking down the explanation logit in parts of (27). In these Figures, CCRC indicates the Concept-Class Relation Coefficient and the *total* equals *sample concept* - *baseline-concept* + *correction*, exactly as in (27), excluding the small residual term.

The concepts that affect the prediction positively the most (Fig. 20) are *batters-box-s* and *stadium-baseball-s* as well as the absence of *train* and *forest-road-s*. As we can see in the Figures, in most cases, e.g. for the concepts *grass-1, batters-box-s, stadium-baseball-s, meshed, martial-arts-gym-s, cavern-indoor-s, tree, forest-road-s,ice-skating-rink-indoor-s* the sign of the difference in concept contribution between the sample and the baseline does not change with the consideration of the correction factor. However, there are some cases in which the imperfect state of convergence when learning the directions has an impact on the quality of the explanation; e.g. for the concepts *grass-2,sky,wall,pool-table,train,highway-s,volleyball-court-outdoor-s,airplane*. In those cases, the consideration of the correction factor changes the sign of the total concept contribution. Many of the cases that fall into this last category exhibit marginal differences in concept contribution scores between the sample and the baseline; for instance: *grass-2, sky, wall, train, airplane*, which could justify, at least partially, this behavior.

7.10 Application: Counterfactual Explanations

In this section, we provide a concrete example of how the learned Encoding-Decoding Direction Pairs can be harnessed in order to provide counter-factual explanations. In this case study, we will be studying ResNet18 trained on Places365 and EDDPs learned with CFM and $I = 512$. We consider the input image depicted in Fig. 21 - left. This image is correctly predicted by the network as *driveway* with confidence 69%. The second image of the same figure depicts a segmentation map of that image based on the learned concept detectors. To keep the visualization simple, we only show the most dominant detected concepts. We explore two interventions in the representation space: a) **concept removal: encoding the absence** of a particular concept in a patch embedding b) **concept addition: encoding the presence** of a particular concept in a patch embedding. For both cases we make use of (20).

To compute target projected values t we use the training split of Broden. When we do concept removal, we choose t to be equal to the lowest 0.005% quantile of projected feature activations on filter $\boldsymbol{w}_i$. Similarly, when we do concept addition, we choose t to be equal to the top 0.005% quantile of projected feature activations. This process ensures that the signal value of $\boldsymbol{x_p}$ for concept i after the intervention matches the signal value of samples with or without the concept.

We consider two counter-factual scenarios. In the first, we study how the prediction would change if the *road* was replaced by a *building*, and second, how the same prediction would change if the *building* was replaced by an *airplane*. To accomplish that, for each scenario, we perform two interventions one after the other: a concept removal followed by a concept addition. In the first scenario, the prediction is changed to *apartment-building-outdoor* with confidence 22%, while in the second, the prediction is changed to *runway* with confidence 57%. (Fig. 21). In both cases, the change in the prediction outcome aligns with human intuition.

7.11 Application: Toy Model Correction

Table 12: Network accuracy and confusion matrix for the network trained on the Chess Pieces dataset. Rows correspond to ground-truth labels and colums to network predictions. Three classes are considered: **b**ishop/k**n**ight/**r**ook. The rows of the confusion matrix are normalized against ground-truth element count. Three datasets are also considered: **Clean** (without watermarks), **Poisoned** (with watermarks) and **Clean & Poisoned** which is the union of the previous two.

Dataset:	**Clean**			**Poisoned**			**Clean & Poisoned**		
Accuracy:	0.93			0.34			0.64		
	b	**n**	**r**	**b**	**n**	**r**	**b**	**n**	**r**
b	0.95	0.05	0.0	0.0	0.0	1.0	0.48	0.02	0.5
n	0	0.95	0.05	0.0	0.0	1.0	0.0	0.48	0.52
r	0.04	0.04	0.92	0.0	0.0	1.0	0.02	0.02	0.96

In this experiment we demonstrate how the proposed approach may be utilized to correct a toy model that relies on controlled confounding factors to make its predictions. For the purposes of this toy experiment we use a small convolutional neural network with 5 `Conv2d` layers each one followed by a `ReLU` activation. The top of the network is comprised of a Global Average Pooling (GAP) layer and a linear head. After each convolutional layer, except the last, there is a `Dropout` layer with $p = 0.3$. All `Conv2d` layers have kernel size 3x3 and stride 2 except the last one which has stride 1. Furthermore, the latent space dimensionality is set to 16 for all convolutional units. We consider the task of predicting the chess piece name from an image depicting the piece. We use the *Chess Pieces* dataset from Kaggle [2] which contains a collection of images depicting chess pieces from various online platforms (i.e., piece images appearing in online play). The spatial resolution of those images is 85x85. For simplicity, we consider 3 chess pieces to be classified by the network, namely: *bishop, knight, rook*, thus the network predicts $K = 3$ output classes. The total number of images in the dataset is 210, 67 for *bishop*, 71 for *knight* and 72 for *rook*. We make a stratified train-test split with the training set ratio set to 0.7. To encourage the model to learn a bias to make its predictions, we poison half of the *rook* images of the training set with the watermark text "rook" on the top left of each rook image. With the introduction of this bias on half of the images, we expect that the network learns that the watermark concept has a positive influence on the *rook* class, while not being the only feature of positive evidence for the same class, since we include rook images in the training set without the watermark.

7.11.1 Network Training and Evaluation

We train the network with cross-entropy loss and the Adam optimizer with learning rate 0.005 for 1000 epochs. In the (poisoned) training set, the model achieves 100% accuracy. For evaluation, we construct three datasets based on the test split that we created earlier. First, we consider a clean test set, a dataset comprised of test images without any watermarks (**Clean**). Second, we consider the previous clean set but with all the images being poisoned with the watermark (**Poisoned**) and c), we consider the union of the previous two datasets (**Clean & Poisoned**). Table 12 summarizes the performance of the network in each one of the three datasets. As evidenced by the *Poisoned* section of the detailed confusion matrix, the watermark is a strong feature that, whenever it is present in the image, directs the prediction towards the *rook* class.

7.11.2 Direction Learning for Watermark Identification

We now consider the application of the proposed method in identifying the watermark direction, from the bottom up, without relying on annotations. As we've shown in the previous sections, the proposed approach

[2] Chess Pieces Dataset (85x85): `https://www.kaggle.com/datasets/s4lman/chess-pieces-dataset-85x85`

is unsupervised and is able to identify directions influential to the model's predictions. Since we already identified that the watermark actually influences the predictions of the network in a consistent manner, we seek to answer the following two research questions: a) can the proposed EDDP method identify the watermark as a concept? That is, is any of the learned classifiers responsible for detecting the watermark? b) Supposing the answer to (a) is positive, given the watermark's concept detector and the respective learned signal vector, can we fix the network in order to not rely on the watermark for its predictions ?

Direction Learning We consider the last convolutional layer as our layer of study. This layer has spatial dimensionality 2x2. To learn the latent directions, we apply our method by following the learning process described in section A.3 and we use the network's training set as our concept dataset. Furthermore, for stable learning, we learn the directions with the Augmented Lagrangian loss scheme of Section 4.5. We optimize $\lambda^{fs}\mathcal{L}^{fs} + \lambda^{cur}\mathcal{L}^{cur}$ with the target constraints $\tau^{ma} = 0.8, \tau^{ic} = 0.01, \tau^{eac} = 0.01, \tau^{mm} = 8.0, \tau^{fso} = 0.1$, and weights $\lambda^{fs} = 2.6$ and $\lambda_{cur} = 0.25$. The most important hyper-parameter to tune is the dimensionality of the concept space I.

Watermark Direction Identification We found that, when learning with $I = 6$, the proposed approach is able to identify the watermark direction. By using the learned classifiers as concept detectors, we are able to group the spatial features of the 2x2 image representations into clusters of the same concept. When applied on an image representation, each learned classifier produces a form of a binary label-map, with each element of the label-map indicating whether the part of the image behind the spatial representation belongs to the concept. In Fig. 22 we provide example image segmentations based on those label-maps. From the qualitative visualizations, we see that classifier 5 identifies the watermark. Although annotations were not required to learn the direction, since this is a controlled experiment and we know in which images we injected the watermark, we are able to quantify how well this classifier can detect the concept by evaluating its IoU performance on the concept dataset. We found that this classifier detects the watermark concept with IoU 0.85.

7.11.3 Influence Testing with RCAV

We use RCAV to measure the sensitivity of the model with respect to the watermark signal vector. The sensitivity scores reported by RCAV are -1 for the classes *bishop* and *knight* while it is 1 for the class *rook*. This implies that when the image has the watermark it becomes more *rook* and less *bishop* or *knight*. This quantitative score aligns with our intuition regarding the watermark.

7.11.4 Signal Vector Faithfulness to the Watermark Concept

Leveraging our knowledge of which images contain the watermark, we can determine the watermark's encoding direction by calculating the watermark's Pattern-CAV (Pahde et al., 2024). Subsequently, we quantify the directional alignment between the Pattern-CAV, which was learned with supervision, and the signal vector, which was learned without. We found that the cosine similarity between these two is 0.99, indicating estimations that agree.

7.11.5 Model Correction by Using the Watermark's Encoding and Decoding Directions

Let $\boldsymbol{w}$ and b denote the learned parameters of the watermark concept detector and $\hat{\boldsymbol{s}}$ denote the respective learned signal vector. Without re-training or fine-tuning the network, we are going to suppress the watermark artifact component from the representation whenever it is detected by the concept detector. We propose the following feature manipulation strategy that we apply at the features of the last convolutional layer.

$$\boldsymbol{x}'_{\boldsymbol{p}} = \mathrm{ReLU}(\boldsymbol{x}_{\boldsymbol{p}} - mk\hat{\boldsymbol{s}}), m = \sigma(\boldsymbol{w}^T \boldsymbol{x}_{\boldsymbol{p}} - b) \tag{33}$$

with k chosen such that $\boldsymbol{w}^T\boldsymbol{x}'_{\boldsymbol{p}} = \mathbb{E}_{\boldsymbol{p}\in\mathcal{N}}[\boldsymbol{w}^T\boldsymbol{x}_{\boldsymbol{p}}]$, $\mathcal{N} = \{\boldsymbol{p} : \boldsymbol{w}^T\boldsymbol{x}_{\boldsymbol{p}} - b < 0\}$; see also (20). This choice of k ensures that the signal value associated with the watermark concept within the patched representation matches the mean value found in the collection of patches lacking the watermark. The ReLU in (33) ensures that the manipulation does not move the features out of the domain of the linear head.

Figure 22: Example image segmentations based on the concept detectors learned for the model correction experiment. Top rows illustrate pictures with the concept and bottom rows illustrate pictures without. Classifier 5 detects the watermark.

7.11.6 Evaluation of the Corrected Model

We evaluate the corrected model according to the same protocol that we did in Section 7.11.1. The results are depicted in Table 13. Compared to the performance of the original network (Table 12), we see that the corrected model: a) has comparable accuracy as the original model on the clean test set b) is significantly more accurate on images of the poisoned dataset with an absolute improvement of +31% and c) performs substantially better on the union of clean and poisoned datasets with an absolute improvement of +14%. We also compare our correction strategy to using a random manipulation direction with the same k as before. (i.e. using a random vector in place of the learned signal vector in (33)). In a series of 10 trial evaluations on the Poisoned Test set, we verified that, in 9 out of 10 cases, **no improvement** was achieved: the classification accuracy was the same as the original model and the confusion matrix was still the same as in Table 12-Middle. The same observation holds when considering the learned filter direction in place of the learned signal vector. The remaining case demonstrated an improvement of +15% which is still inferior to +31% when using the signal vector.

Table 13: Network accuracy and confusion matrix for the **corrected** network trained on the Chess Pieces dataset. Rows correspond to ground-truth labels and columns to network predictions. Three classes are considered: **b**ishop/k**n**ight/**r**ook. The rows of the confusion matrix are normalized against ground-truth element count. Three datasets are considered: **Clean** (without watermarks), **Poisoned** (with watermarks) and **Clean & Poisoned** which is the union of the previous two.

Dataset:	**Clean**			**Poisoned**			**Clean & Poisoned**		
Accuracy:	0.92 (-1%)			0.65 (+31%)			0.78 (+14%)		
	b	**n**	**r**	**b**	**n**	**r**	**b**	**n**	**r**
b	0.95	0.05	0.0	0.5	0.2	0.3	0.73	0.12	0.15
n	0.0	1.0	0.0	0.14	0.72	0.14	0.07	0.86	0.07
r	0.05	0.13	0.82	0.05	0.22	0.73	0.05	0.18	0.77

8 Limitations

Our method builds on the linear representation hypothesis, assuming that concepts are encoded as directions in the latent space. While this view aligns with several prior works, alternative formulations such as multidimensional concept discovery (Vielhaben et al., 2023) or linear subspaces (Chormai et al., 2024) exist but fall outside the scope of our study. Additionally, we constrain our experiments to settings where the number of discovered concepts is smaller than the embedding dimensionality. As such, we do not compare with methods like Sparse Autoencoders (SAEs) (Lim et al., 2024; Cunningham et al., 2024; Sharkey et al., 2022) that assume an overcomplete representation. Even though we restricted our experiments as such, future studies may consider this analysis, since our method is not technically limited in this regard. While we evaluated our approach across multiple CNN architectures, we did not investigate applications to Vision Transformers (ViTs) (Caron et al., 2021; He et al., 2022), despite existing literature suggesting that similar linear assumptions may apply in that context (Kaltampanidis et al., 2025)—this remains a promising direction for future work. Moreover, unlike some unsupervised baselines that operate on class-specific image subsets constructed from model predictions, we applied our method to unlabeled data without class filtering, due to the lack of dense annotations in the training sets. Nevertheless, our framework could, in principle, be adapted for class-conditional analysis. Finally, our study aimed to minimize hyperparameter tuning by relying on prior work (Doumanoglou et al., 2023; 2024) and empirical preliminary experiments; however, further tuning or exploration of additional hyperparameters may yield improvements in clustering quality, interpretability, or influence (Section A.8).

9 Conclusion

We introduced an innovative unsupervised technique to uncover pairs of latent space encoding-decoding directions that align with interpretable concepts of influence. This research offers a new perspective on the unsupervised identification of concept directions, unlike previous methods which are based on feature reconstruction or matrix decomposition. We believe that our work opens the door to richer model diagnostics, fine-grained explanations, and targeted interventions, paving the way for future research on scalable concept discovery, dynamic model editing, and integration into decision-making systems.

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A Appendix

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A.1 Unsupervised Interpretable Basis Extraction and Concept-Basis Extraction Losses

This Section complements Section 3.3 by providing further details on the loss terms of Unsupervised Interpretable Basis Extraction (UIBE) (Doumanoglou et al., 2023) and Concept Basis Extraction (CBE) (Doumanoglou et al., 2024).

Sparsity Loss ($\mathcal{L}^s$) (Doumanoglou et al., 2023) Based on the observation that the number of semantic labels that may be attributed to an image patch is only a fraction of the set of possible semantic labels, this loss enforces sparsity on the number of concepts that may be attributed to a patch embedding. In particular, the sparsity loss for pixel $\boldsymbol{p}$ is based on minimizing entropy and is defined as:

$$\mathcal{L}^s_{\boldsymbol{p}} = -\sum_i q_{\boldsymbol{p},i} \log_2 q_{\boldsymbol{p},i}, \quad q_{\boldsymbol{p},i} = \frac{y_{\boldsymbol{p},i}}{\sum_i y_{\boldsymbol{p},i}} \tag{34}$$

The aggregated sparsity loss $\mathcal{L}^s$ is:

$$\mathcal{L}^s = \mathbb{E}_{\boldsymbol{p}}\big[\mathcal{L}^s_{\boldsymbol{p}}\big] \tag{35}$$

Maximum Activation Loss ($\mathcal{L}^{ma}$) (Doumanoglou et al., 2023)

With the complement of this loss, the cluster membership variables $y_{\boldsymbol{p},i}$ are enforced to become binary:

$$\mathcal{L}^{ma} = \mathbb{E}_{\boldsymbol{p}}\Big[-\sum_i q_{\boldsymbol{p},i} \log_2 y_{\boldsymbol{p},i}\Big] \tag{36}$$

Inactive Classifier Loss ($\mathcal{L}^{ic}$) (Doumanoglou et al., 2024)

This loss ensures that each concept detector in the set classifies positively at least $\nu \in [0, 1]$ percent of pixels in the concept dataset, avoiding clusters with few assignments.

$$\mathcal{L}^{ic} = \mathbb{E}_i\Big[\frac{1}{\nu}\mathrm{ReLU}\big(\nu - \mathbb{E}_{\boldsymbol{p}}[y^{\gamma}_{\boldsymbol{p},i}]\big)\Big] \tag{37}$$

with $\nu = \frac{\tau}{I}$, $\gamma > 1, \gamma \in \mathbb{R}^+$ denoting a sharpening factor and $\tau \in [0, 1]$ denoting a percent of pixels in the dataset to be evenly distributed among the I classifiers in the set.

Maximum Margin Loss ($\mathcal{L}^{mm}$) In the original formulation of Doumanoglou et al. (2023), the Maximum Margin Loss was defined as $\mathcal{L}^{mm} = \frac{1}{M}$ with M being a single parameter for the whole set of classifiers since the optimization was performed in the standardized space with shared parameters for the margins M and biases b. In this work, we removed the standardized space constraints and instead, we have a margin parameter M_i for each classifier in the set. Thus, we modify the Maximum Margin loss to become:

$$\mathcal{L}^{mm} = \frac{1}{I} \sum_i \frac{1}{M_i} \tag{38}$$

A.2 Theoretical Comparison with Concept-Basis Extraction

To improve the interpretability of the discovered directions, Doumanoglou et al. (2024) made a first attempt to exploit the knowledge encoded in the network, through feature manipulation. In particular, it was suggested that uncertain network predictions shall occur when there is no positive concept content in the features. This previous approach is similar to ours in the sense that it uses feature manipulation and subsequent entropy maximization on the network's prediction outcomes. Yet, the fundamental difference with what we propose here lies within the feature manipulation strategy. This previous approach suggested that representations $\boldsymbol{x_p}$ should be manipulated towards the concept detectors' hyperplanes, **only for the concepts that are present in** $\boldsymbol{x_p}$ (i.e. manipulating towards the **negative** direction of the filter weights, when the respective concept detectors classify $\boldsymbol{x_p}$ positively). Features **were not manipulated** in the direction of the weights to bring them towards the separating hyperplane, when they lie in the subspace of negative concept classification. While this previous attempt tried to exploit the uncertainty region of the model, it was essentially suggested that the network's predictions should be uncertain when for all $\boldsymbol{x_p}$, none of the classifiers makes positive predictions, without minding about confident negative ones. This is fundamentally different from what we propose in the present work, as here we suggest that uncertain network predictions are linked to uncertain concept information. We enforce the latter **by manipulating all all features towards the hyperplanes**, regardless of whether features were positively or negatively classified for the presence of a concept. We once again emphasize that here we suggest that the network's predictions should be maximally uncertain when for all $\boldsymbol{x_p}$ none of the classifiers makes confident predictions, either positive **or negative**. Additionally, in Doumanoglou et al. (2024), signal directions were completely overlooked.

A.3 Direction Learning Process

We learn the directions of the proposed method in a four-step process: a) we first learn the parameters $\boldsymbol{w}_i, b_i$ following Doumanoglou et al. (2024), replacing the *CNN Classifier Loss* with the proposed $\mathcal{L}^{uur}$; b) we then continue optimizing $\boldsymbol{w}_i, b_i$, removing the orthogonality and standardization constraints while keeping $\mathcal{L}^{uur}$ and incorporating the additional losses from Section 4.2; c) next, we learn the signal vectors using the filters of the learned classifiers as regressors in (1) to initialize $\{\hat{\boldsymbol{S}}\}$; and d) finally, we jointly optimize $\hat{\boldsymbol{s}}_i$, $\boldsymbol{w}_i, b_i$, using all previous losses, replacing $\mathcal{L}^{uur}$ with $\mathcal{L}^{cur}$ and adding $\mathcal{L}^{fso}$ from Sections 4.3 and 4.4.

A.4 Details for the Experiment on Synthetic Data

We train the network using cross-entropy loss and the Adam (Kingma, 2014) optimizer, with learning rate 0.0005 and batch size 1024 for 4000 epochs. In principle, we follow the process defined in Section A.3, but due to the simplicity of the example, during (a) we don't use $\mathcal{L}^{uur}$, we omit step (b) and proceed directly from (a) to (c). In both steps (a) and (d) we use the Augmented Lagrangian Loss, the Adam optimizer, and the Cosine Annealing learning rate scheduler (Loshchilov & Hutter, 2016). In step (a), we omit the constraints of the Augmented Lagrangian loss that are not applicable. The Augmented Lagrangian formulation greatly stabilizes learning and avoids local optima. For step (a) we solve the constrained optimization problem of minimizing $\mathcal{L}^s$ with $\tau^{ma} = 0.8$, $\tau^{mm} = 5$ and $\tau^{ic} = 0.0$. For step (d) we minimize $\lambda^{fs}\mathcal{L}^{fs} + \lambda^{cur}\mathcal{L}^{cur}$ with

Table 14: Left: Data matrices $\boldsymbol{S}$ and $\boldsymbol{D}$ for the experiment on synthetic data. Right: Cosine similarities for every pair of vectors in $\boldsymbol{S}$, $\boldsymbol{D}$, i.e.: $\boldsymbol{C}^T\boldsymbol{C}, \boldsymbol{C} = [\boldsymbol{S}|\boldsymbol{D}]$.

$\boldsymbol{S}$			$\boldsymbol{D}$	
0.6368	0.8583	0.5259	0.4008	0.6659
0.1561	-0.3371	0.1561	0.4585	0.6038
0.1633	-0.1533	0.7557	0.3337	-0.2065
0.2617	0.1643	-0.1580	0.5797	-0.2154
0.6226	-0.1607	-0.1643	-0.1596	0.1687
-0.1759	0.1607	-0.1594	0.2744	0.1617
-0.1592	0.1531	-0.1567	0.2232	0.1567
-0.1760	0.1554	-0.1612	0.1763	0.1546

Cosine-Similarities				
1.0	0.3319	0.4204	0.3188	0.4526
0.3319	1.0	0.2087	0.3649	0.4111
0.4204	0.2087	1.0	0.3621	0.2195
0.3188	0.3649	0.3621	1.0	0.4296
0.4526	0.4111	0.2195	0.4296	1.0

$\tau^{ma} = 0.5$, $\tau^{mm} = 15$, $\tau^{ic} = 0.0$, $\tau^{eac} = 0.0$, $\tau^{fso} = 0.01$. The learning rate we use for step (a) is 0.00025 and for step (b) is 0.0005. The number of learning epochs is set to 10000 and 20000, for each step respectively. For the loss weights we use $\lambda^{fs} = 2.6$ and $\lambda^{ur} = 0.25$. The sharpening factor γ of $\mathcal{L}^{ic}$ is set to $\gamma = 2.0$, the τ hyperparameter of the same loss is set to $\tau = 1.0$, the ν sharpening factor of $\mathcal{R}_{SW}$ to $\nu = 2.0$, the ρ of $\mathcal{L}^{eac}$ is set to $\rho = 5/3$ and the μ sharpening factor of $\mathcal{L}^{fs}$ is set to 2.0.

The specific values of matrices $\boldsymbol{S}$ and $\boldsymbol{D}$ used in this experiment, and the cosine similarities between every pair of vectors, are provided in Table 14.

A.5 Extracting Signal Values with the Filters of Concept Detectors

As discussed in Section 4.3, signal values, which are required to estimate the encoding direction of a concept, are extracted using the filter weights of the concept detectors. Yet, as we discussed in that Section, in order for this to happen, the filter weights $\boldsymbol{w}_i$ need to be orthogonal to $\boldsymbol{s}_j$ and $\boldsymbol{D}$. Since we do not explicitly estimate distractors in this work, there may be an inevitable error when extracting the value of the signal (we say maybe, because this might also be mitigated by the Uncertainty Region Alignment losses or filters converge to become perpendicular to distractors due to the fact that they contain information independent of concept content). Here we study on the order of this error. From 3 we have:

$$\boldsymbol{x_p} = \boldsymbol{S}\boldsymbol{\alpha_p} + \boldsymbol{D}\boldsymbol{\beta_p} + \boldsymbol{c}$$

When extracting the signal value with a filter, the estimation becomes:

$$\begin{aligned} z_{\boldsymbol{p}} = \boldsymbol{w}_i^T\boldsymbol{x_p} = \boldsymbol{w}_i^T\boldsymbol{S}\boldsymbol{\alpha_p} + \boldsymbol{w}_i^T\boldsymbol{D}\boldsymbol{\beta_p} + \boldsymbol{w}_i^T\boldsymbol{c} \\ \frac{z_{\boldsymbol{p}}}{\boldsymbol{w}_i^T\boldsymbol{s}_i} = a_{\boldsymbol{p},i} + \frac{\boldsymbol{w}_i^T\boldsymbol{D}\boldsymbol{\beta_p}}{\boldsymbol{w}_i^T\boldsymbol{s}_i} + \frac{\boldsymbol{w}_i^T\boldsymbol{c}}{\boldsymbol{w}_i\boldsymbol{s}_i} \end{aligned} \tag{39}$$

From (39) and as we've already seen in (14), we notice that the latent space bias $\boldsymbol{c}$ introduces an additional constant error term when estimating the signal values. In the real-world scenario when this $\boldsymbol{c}$ is not known, we can use the following estimator $\hat{a}_{\boldsymbol{p},i}$ which depends on the average of features $\boldsymbol{x_p}$:

$$\begin{aligned} \hat{a}_{\boldsymbol{p},i} &= \frac{\boldsymbol{w}_i^T\boldsymbol{x_p}}{\boldsymbol{w}_i^T\boldsymbol{s}_i} - \frac{\boldsymbol{w}_i^T\mathbb{E}_{\boldsymbol{p}}[\boldsymbol{x_p}]}{\boldsymbol{w}_i^T\boldsymbol{s}_i} = \\ \hat{a}_{\boldsymbol{p},i} &= \frac{\boldsymbol{w}_i^T\boldsymbol{x_p}}{\boldsymbol{w}_i^T\boldsymbol{s}_i} - \frac{\boldsymbol{w}_i^T\boldsymbol{s}_i\mathbb{E}_{\boldsymbol{p}}[a_{\boldsymbol{p},i}]}{\boldsymbol{w}_i^T\boldsymbol{s}_i} - \frac{\boldsymbol{w}_i^T\boldsymbol{D}\mathbb{E}_{\boldsymbol{p}}[\boldsymbol{\beta_p}]}{\boldsymbol{w}_i^T\boldsymbol{s}_i} \\ \hat{a}_{\boldsymbol{p},i} &= a_{\boldsymbol{p},i} - \mathbb{E}_{\boldsymbol{p}}[a_{\boldsymbol{p},i}] + \frac{\boldsymbol{w}_i^T\boldsymbol{D}}{\boldsymbol{w}_i^T\boldsymbol{s}_i}(\boldsymbol{\beta_p} - \mathbb{E}_{\boldsymbol{p}}[\boldsymbol{\beta_p}]) \end{aligned} \tag{40}$$

The latter is an estimator of $a_{\boldsymbol{p},i}$ with respect to the mean $\mathbb{E}_{\boldsymbol{p}}[a_{\boldsymbol{p},i}]$ and with an error term depending on distractors, irrespective of constant bias.

Table 15: Hyper-parameters used to learn the Direction Pairs

ResNet18 / Places365			
I	Step	Epochs	LR
384/448/512	a	500	0.005
384/448/512	b	2500	0.00025
384/448/512	d	1250	0.00005
EfficientNet / ImageNet			
I	Step	Epochs	LR
960/1120/1280	a	800	0.001
960/1120/1280	b	3500	0.00005
960/1120/1280	d	1750	0.00005

ResNet50 / MiT			
I	Step	Epochs	LR
1536/1792/2048	a	1300	0.001
1536/1792/2048	b	2600	0.00025
1536/1792/2048	d	1300	0.0001
VGG16 / ImageNet			
I	Step	Epochs	LR
384/448/512	a	1000	0.001
384/448/512	b	1000	0.0001
384/448/512	d	500	0.0001

Inception-v3 / ImageNet			
I	Step	Epochs	LR
1536/2048	a	1500	0.001
1536/1792/2048	b	3000	0.00005
1536/1792/2048	d	1500	0.00005
1792	a	1500	0.01

A.6 Details on the Faithfulness Assessment of Encoding-Decoding Direction Pairs

Due to the considerable computational load required to conduct this experiment, we make some simplifications. First, we consider a subset of the learned direction pairs by randomly choosing 100. Candidate pairs are the ones with a concept detector that is considered interpretable by Network Dissection (i.e. the detector exhibits an IoU performance greater than 0.04 when detecting the concept). Second, to construct the image set that contains the concept, we consider 10 unique images within the set of the most confident (patch-level) predictions of the concept detector. For each image, we run the deep dream optimization for $K = 40$ iterations, and we record the patch embeddings (feature activations) containing the concept with an interval of 5 steps. For dreaming, we don't use zooming, but we do use the robustness transforms originally proposed in Olah et al. (2017). Regarding the line fitting process, we consider a parametric line as $\boldsymbol{c} + \lambda \boldsymbol{d}$, $\lambda \in \mathbb{R}$, with $\boldsymbol{c} \in \mathbb{R}^D$ denoting the line's origin and $\boldsymbol{d} \in \mathbb{R}^D$ its direction (the *dreaming* direction). At the end of the dreaming optimization loop and after recording the feature activations of the concept, we minimize the average distance from each feature to the line. Finally, we make sure that the dreaming direction points towards the direction of feature evolvement across iterations by considering making a sign flip, i.e. multiplying $\boldsymbol{d}$ with -1.

A.7 Details for the Experiments on Deep Image Classifiers

Learning Details In Table 15 we provide the main hyper-parameters to train the direction pairs for each step. The learning rate that we provide (LR) is considered as the reference learning rate for a batch size of 4096. In practice, we scale both the learning rate and the batch size based on the available GPU memory and the number of GPUs. We use the Adam Kingma (2014) optimizer and the cosine annealing learning rate scheduler (Loshchilov & Hutter, 2016). While for step (a) we follow the hyper-parameter setup of Doumanoglou et al. (2024), for steps (b) and (d) we make different choices. For $\mathcal{L}^{ic}$ and $\mathcal{L}^{eac}$ we set their hyper-parameters τ and ρ as follows: For ResNet18 and VGG16, τ and ρ are set such that the minimum cluster size is equal to 400 and the maximum 50000. For EfficientNet and Inception-v3, the same numbers are 520 and 65000, while for ResNet50 the minimum cluster size is set to 920 and the maximum to 75000. These are all set based on the statistics of the concept datasets. The μ sharpening factor of $\mathcal{L}^{fs}$ and the ν sharpening factor of $\mathcal{R}_{SW}$ are set to 2.0.

For Augmented Lagrangian Loss, in all cases we used the following hyper-parameters: $\lambda^{fs} = 2.6$, $\lambda^{ur} = 0.25$, $\tau^{ma} = 0.8$, $\tau^{ic} = 0$,$\tau^{eac} = 0$,$\tau^{fso} = 0.01$. For ResNet18, EfficientNet and VGG16 we use $\tau^{mm} = 5.0$, while for Inception-v3 and ResNet50 we used $\tau^{mm} = 6.0$.

When using $\mathcal{L}^{uur}$ and $\mathcal{L}^{cur}$, we observed better results when manipulating features with a stochastic magnitude in the direction $\boldsymbol{dx_p}$, i.e. shifting representations as $\boldsymbol{x}'_{\boldsymbol{p}} = \boldsymbol{x_p} - \kappa \boldsymbol{dx_p}$ with κ a random number in $[0.1, 0.5]$. In practice, we separate filter directions from their magnitude $1/M_i$ and learn them independently

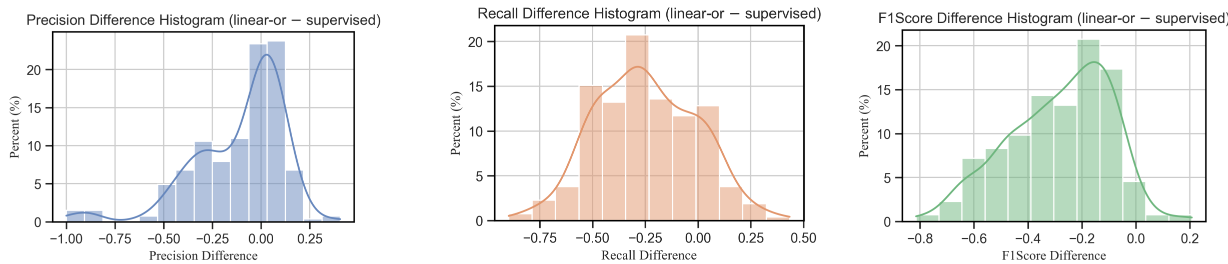


Figure 23: Interpretability Comparison. Histogram of differences in binary metrics: Precision, Recall, F1Score between the *Linear-OR* set of concept detectors learned with EDDP-C, $I = 512$, and classifiers learned in a supervised way (IBD Zhou et al. (2018)). The network here is ResNet18 trained on Places365.

as suggested in Doumanoglou et al. (2024). For enforcing $||\boldsymbol{w}_i||_2 = 1$ (i.e. unit norm filter vectors) we use parametrization on the unit hyper-sphere.

Details on Datasets used to Compute Concept Sensitivity with RCAV To conduct concept sensitivity testing with RCAV we need access to a labeled dataset coming from the domain of the model. In practice, it is common to use the validation split of the dataset used to train the model. To mitigate the required computation time, we limited the size of the validation datasets as follows: For ImageNet, we used the validation split of ImageNet-S-300 Gao et al. (2022), and for Moments-in-Time, we considered Moments-In-Time Mini. Since Moments-In-Time is a video dataset, but the model that we studied works in the image domain, we constructed an image dataset by sampling 3 frames equally apart from each video (i.e. the first, the mid, and the last frame of the video). For Places365, we didn't make a size reduction as the validation split of the dataset was manageable with our resources.

Details on RCAV's Statistical Significance Test In all experiments, we set RCAV's perturbation hyperparameter, to $\alpha = 5$. For direction significance testing, we use RCAV's label permutation test. To construct random noise signal vectors, we (a) construct a dataset of feature-(binary) label pairs based on the decision rule of each one of the concept detectors. To deal with great class imbalance, we construct a pool of negative samples that is at most 20 times more than the positive ones; (b) we construct N noisy versions of that dataset by label permutation; (c) we learn a noise-classifier to distinguish features based on the permuted labels, and (d) we concurrently estimate a noise-signal vector using (1) and the subsampling process described in Section 4.3. To learn each one of the noise signal vectors, and before permuting the labels, we construct a balanced dataset of at most 5000 samples, picked randomly from the pool. We train the noise classifiers using Adam for 100 epochs and a learning rate 0.01. By using noise signal vectors as RCAV's noisy directions, and with the number of those vectors per classifier set to $N = 100$, we subsequently calculate RCAV's p-values. We apply Bonferroni correction to all p-values by dividing the significance threshold 0.05 by the number of concept detectors I and the number of model classes.

Learning Details for NMF When learning directions with NMF, we used the implementation found in Yu (2020). To make computations manageable, we reduce the spatial dimensionality of image representations by applying Adaptive Average Pooling to a (2,2) resolution, in a similar way as it was done in Fel et al. (2023c). In all cases, we learn the NMF decomposition by running the algorithm for 100000 iterations.

Details for Comparing with the Supervised Approach When learning directions with IBD, for each concept, a dataset is assembled that includes up to 20 times more negative samples than positive ones to address the significant imbalance. Additionally, we use hard negative mining as originally suggested in Zhou et al. (2018).

Figure 23 plots a histogram of classification metric differences between the *Linear-OR* set of classifiers and the classifiers learned in a supervised way. The differences are based on the concept labels, effectively taking the difference of metrics that regard two classifiers (the first from the *Linear-OR* set and the second from Zhou et al. (2018)) with the same concept name.

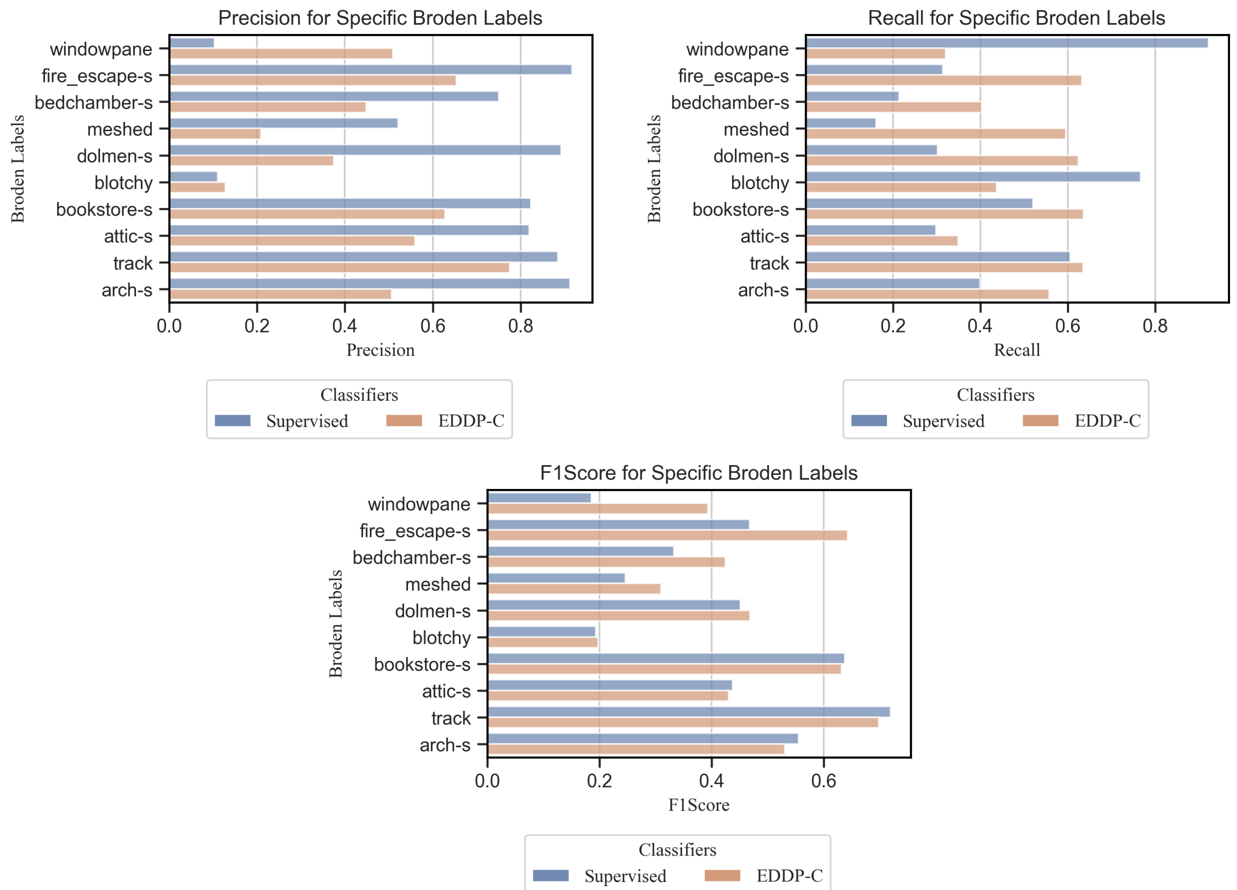


Figure 24: Interpretability Comparison. Exact Precision/Recall/F1Scores for specific concepts in Broden: comparison between the *Linear-OR* set of classifiers learned with EDDP-C, $I = 512$, and classifiers learned in a supervised way (IBD Zhou et al. (2018)). The network here is ResNet18 trained on Places365.

Figures 24, 25, 26 depict concrete binary classification metrics for some of the concept detectors in the *Linear-OR* set of classifiers, comparing them with concept detectors learned with supervision.

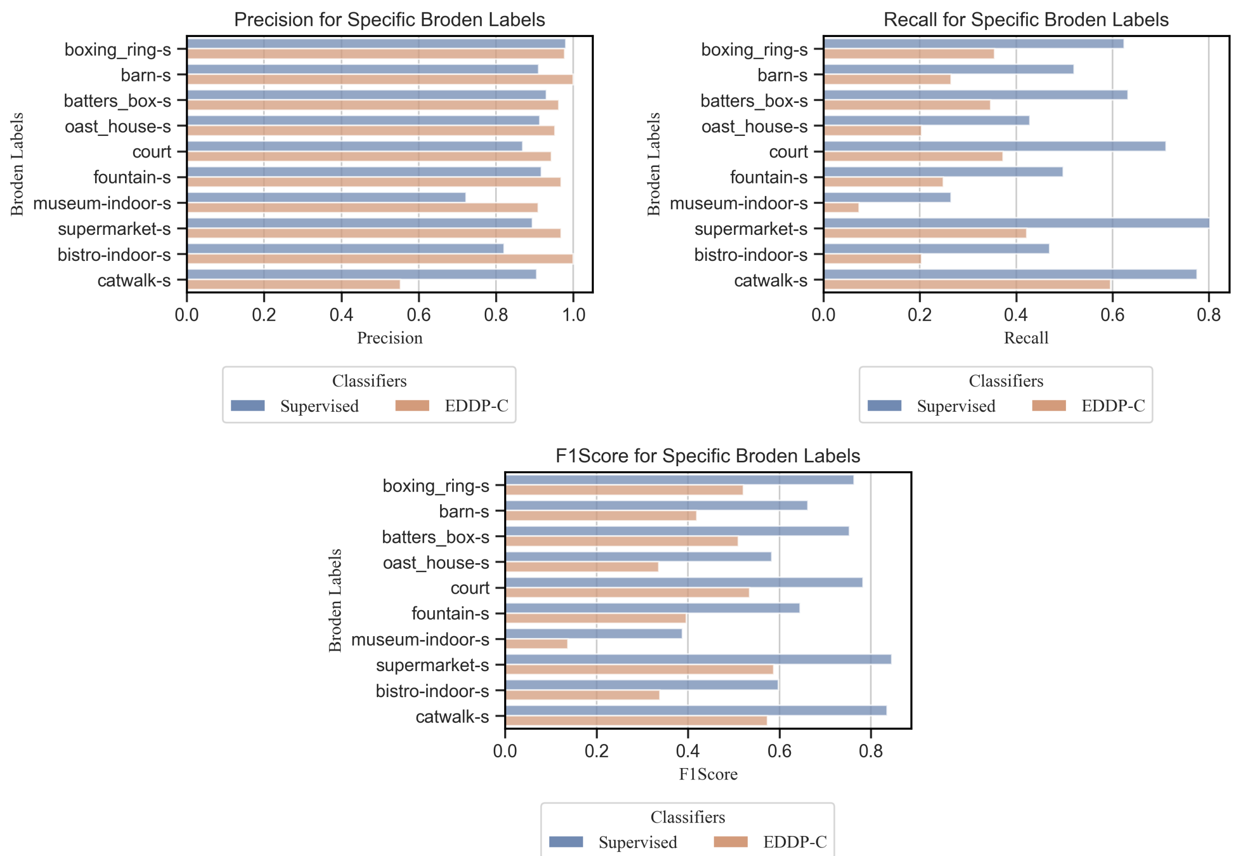


Figure 25: Interpretability Comparison. Exact Precision/Recall/F1Scores for specific concepts in Broden: comparison between the *Linear-OR* set of classifiers learned with EDDP-C, $I = 512$, and classifiers learned in a supervised way (IBD Zhou et al. (2018)). The network here is ResNet18 trained on Places365.

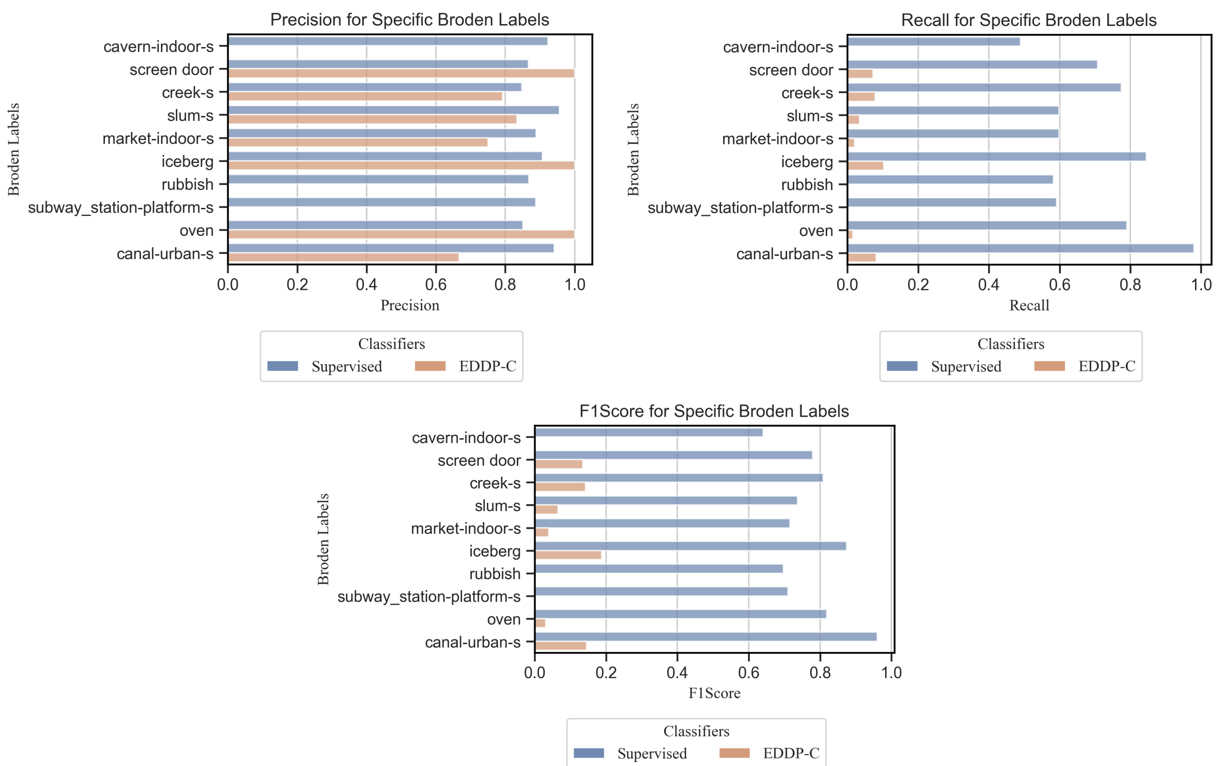


Figure 26: Interpretability Comparison. Exact Precision/Recall/F1Scores for specific concepts in Broden: comparison between the *Linear-OR* set of classifiers learned with EDDP-C, $I = 512$, and classifiers learned in a supervised way (IBD Zhou et al. (2018)). The network here is ResNet18 trained on Places365.

A.8 Hyper-Parameter Study with Respect to Target Separation Margin

Table 16: Comparing EDDP variants based on varying target margin loss τ^{mm}. The network here is ResNet18 trained on Places365 and $I = 448$.

ResNet18 / Places365											
Method	τ^{mm}	Coverage ↑	Redundancy ↓	Precision ↑	Recall ↑	F1 ↑	AP ↑	$\mathcal{M}$ ↓	$\mathcal{S}^1$ ↑	$\mathcal{S}^2$ ↑	mIoU ↑
EDDP-U	4.0	0.85	**1.27**	0.82±0.21	**0.23±0.18**	**0.32±0.19**	**0.54±0.19**	**6.62**	45.92	32.29	**0.12**
EDDP-U	5.0	**0.86**	1.32	**0.83±0.19**	0.22±0.16	**0.32±0.18**	0.53±0.19	6.64	47.5	32.07	0.11
EDDP-U	6.0	**0.86**	1.32	**0.83±0.2**	0.21±0.15	0.31±0.17	0.52±0.19	6.7	**48.84**	**32.44**	0.11
EDDP-C	4.0	**0.86**	**1.27**	**0.83±0.21**	**0.22±0.17**	**0.31±0.19**	**0.52±0.2**	**6.67**	44.71	**31.73**	**0.11**
EDDP-C	5.0	**0.86**	1.33	0.82±0.2	0.21±0.16	**0.31±0.18**	0.49±0.19	6.72	46.3	31.34	0.11
EDDP-C	6.0	**0.86**	1.31	**0.83±0.2**	0.2±0.15	0.29±0.17	0.5±0.18	6.75	**46.01**	30.97	0.1

Table 17: Comparing EDDP variants based on varying target margin loss τ^{mm}. The network here is EfficientNet trained on ImageNet and $I = 1120$.

EfficientNet / ImageNet											
Method	τ^{mm}	Coverage ↑	Redundancy ↓	Precision ↑	Recall ↑	F1 ↑	AP ↑	$\mathcal{M}$ ↓	$\mathcal{S}^1$ ↑	$\mathcal{S}^2$ ↑	mIoU ↑
EDDP-U	4.0	**0.85**	**1.54**	**0.77±0.22**	**0.22±0.18**	**0.3±0.19**	**0.42±0.19**	6.74	**37.45**	**23.0**	**0.03**
EDDP-U	5.0	**0.85**	1.61	0.76±0.21	0.2±0.17	0.28±0.17	0.39±0.17	6.73	31.36	16.54	**0.03**
EDDP-U	6.0	**0.85**	1.6	0.76±0.21	**0.22±0.17**	**0.3±0.17**	0.39±0.17	**6.72**	30.46	16.09	**0.03**
EDDP-C	4.0	**0.85**	**1.52**	**0.77±0.22**	**0.22±0.18**	**0.3±0.19**	**0.42±0.19**	6.79	**34.93**	**22.28**	**0.03**
EDDP-C	5.0	**0.85**	1.54	0.74±0.22	0.2±0.18	0.28±0.19	0.39±0.17	**6.74**	28.62	16.38	**0.03**
EDDP-C	6.0	**0.85**	1.57	0.75±0.21	0.21±0.18	0.29±0.17	0.39±0.17	6.77	28.24	16.19	**0.03**

Tables 16 and 17 consider varying the target margin τ^{mm} when learning EDDP. For EfficientNet, increasing the target classification margin (i.e. the linear separability of patch embeddings) leads to a substantial improvement in both $\mathcal{S}^1$ and $\mathcal{S}^2$ for both EDDP-C and EDDP-U. We stress the fact that increasing the margin is accomplished by decreasing τ^{mm}, as the margin is inversely proportional to the target loss. For ResNet18, the results are more mixed: for EDDP-U, decreasing the margin improves $\mathcal{S}^1$ and $\mathcal{S}^2$, while for EDDP-C there is an improvement in $\mathcal{S}^1$ but at the cost of a slightly inferior $\mathcal{S}^2$ score. We emphasize that when $\tau^{mm} = 4.0$, the results for EfficientNet are substantially better than the metrics we reported in the main body of the paper, for which we used $\tau^{mm} = 5.0$ (Section A.7).

A.9 Additional Experiments on the Faithfulness Assessment of the Encoding-Decoding Direction Pairs

Figures 27 and 28 complement the experiments presented in Figures 11 and 12 for the remaining combinations regarding $\mathcal{L}^{fso}$. Even though less prominent in ResNet18, together with Section 7.2 the experiments sufficiently support that $\mathcal{L}^{fso}$ pushes the distribution of cosine similarities between dreaming directions and signal vectors to become more bell-shaped. Overall, the experiments in this section, similar to the experiments presented in Section 7.2, indicate that in approximately 90% of the cases, these cosine similarities exceed 0.7. In a less rigorous but more qualitative sense, we found that when learning EDDP with $\mathcal{L}^{fso}$, this loss converges to values close to ≈ 0.02, whereas measuring the loss value for a direction set learned without $\mathcal{L}^{fso}$ often leads to a value close to ≈ 0.1, which is still not that far from indicating orthogonality between filters and signal vectors.

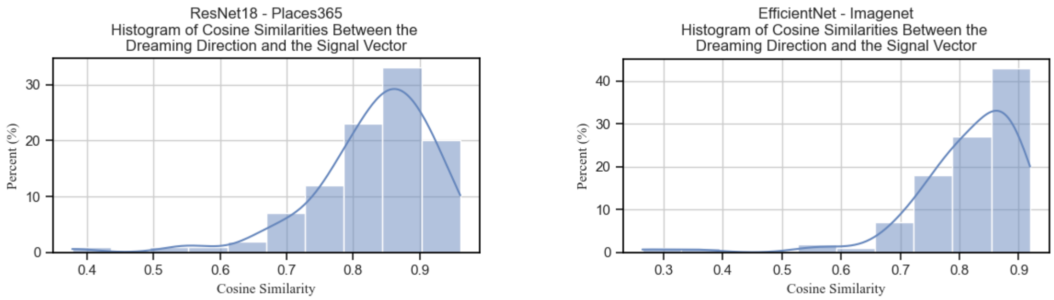


Figure 27: Cosine similarity histogram between *dreaming directions* and *signal vectors*. **Left:** Directions learned for ResNet18 trained on Places365 ($I = 448$). **Right**: Directions learned for EfficientNet trained on ImageNet ($I = 1120$). These histograms regard directions learned **with** $\mathcal{L}^{cur}$ but **without** $\mathcal{L}^{fso}$.

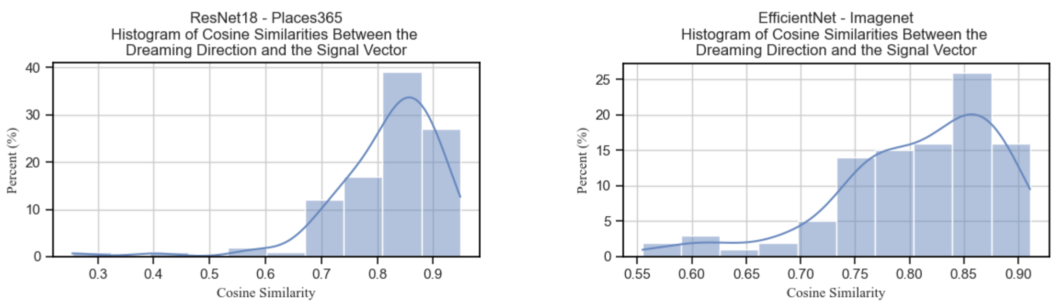


Figure 28: Cosine similarity histogram between *dreaming directions* and *signal vectors*. **Left:** Directions learned for ResNet18 trained on Places365 ($I = 448$). **Right**: Directions learned for EfficientNet trained on ImageNet ($I = 1120$). These histograms regard directions learned with $\mathcal{L}^{uur}$ **and** $\mathcal{L}^{fso}$.

A.10 Ablation Study with Respect to Filter-Signal Orthogonality Loss

Table 18: Ablation study of the method with respect to Uncertainty Region Alignment Losses $\mathcal{L}^{uur}, \mathcal{L}^{cur}$ and the use of Filter-Signal Orthogonality Loss $\mathcal{L}^{fso}$. The network here is ResNet18 trained on Places365.

						ResNet18 / Places365								
I	$\mathcal{L}^{uur}$	$\mathcal{L}^{cur}$	$\mathcal{L}^{fso}$	Coverage ↑	Redundancy ↓	Precision ↑	Recall ↑	F1 ↑	AP ↑	$\mathcal{M}$ ↓	$\mathcal{S}^1$ ↑	$\mathcal{S}^2$ ↑	mIoU ↑	$\mathcal{I}^1$ ↑
384	✓	✗	✗	**0.86**	1.29	**0.82±0.21**	**0.23±0.16**	**0.33±0.18**	**0.53±0.19**	**6.61**	**41.73**	**28.01**	**0.12**	0.58
	✗	✓	✗	**0.86**	**1.26**	**0.82±0.22**	0.22±0.16	0.32±0.18	0.52±0.19	6.62	40.43	27.17	**0.12**	0.6
	✓	✗	✓	**0.86**	1.3	0.81±0.21	**0.23±0.16**	**0.33±0.17**	0.52±0.19	6.65	41.43	27.58	**0.12**	**0.61**
	✗	✓	✓	**0.86**	1.32	0.81±0.21	**0.23±0.16**	**0.33±0.17**	0.5±0.19	6.67	41.5	27.49	**0.12**	**0.61**
448	✓	✗	✗	**0.86**	1.32	**0.83±0.19**	**0.22±0.16**	**0.32±0.18**	**0.53±0.19**	**6.64**	47.5	**32.07**	**0.11**	0.59
	✗	✓	✗	**0.86**	**1.29**	**0.83±0.19**	0.21±0.16	0.3±0.18	0.52±0.19	6.66	45.21	31.1	**0.11**	0.6
	✓	✗	✓	**0.86**	1.33	0.82±0.2	**0.22±0.16**	**0.32±0.18**	0.51±0.19	6.68	**47.57**	31.95	**0.11**	**0.61**
	✗	✓	✓	**0.86**	1.33	0.82±0.2	0.21±0.16	0.31±0.18	0.49±0.19	6.72	46.3	31.34	**0.11**	**0.61**
512	✓	✗	✗	**0.86**	1.28	**0.82±0.22**	**0.21±0.17**	**0.31±0.19**	**0.51±0.21**	**6.66**	**52.51**	**37.78**	**0.11**	0.61
	✗	✓	✗	0.85	**1.23**	**0.82±0.23**	**0.21±0.17**	0.3±0.19	**0.51±0.2**	6.67	50.63	37.35	0.1	0.62
	✓	✗	✓	**0.86**	1.3	**0.82±0.21**	**0.21±0.17**	**0.31±0.19**	0.48±0.2	6.72	52.3	37.71	0.1	0.62
	✗	✓	✓	**0.86**	1.28	0.81±0.24	0.2±0.16	0.29±0.19	0.47±0.2	6.73	50.29	36.99	0.1	**0.63**

In this Section we conduct a detailed ablation study with respect to the use of Filter-Signal Orthogonality Loss ($\mathcal{L}^{fso}$) that was introduced in Section 4.3. In Section A.9 we discussed the impact of $\mathcal{L}^{fso}$ on the faithfulness of the direction pairs, while in this Section we discuss the effects of $\mathcal{L}^{fso}$, in interpretability and influence terms. Tables 18, 19, 20, 21, 22, 23 depict results in terms of interpretability and influence metrics.

The main observations can be summarized to the following: a) When $\mathcal{L}^{fso}$ is not used, using any of the two Uncertainty Region Alignment variants, in the majority of the cases, results in comparable sets of directions, with $\mathcal{L}^{uur}$ typically leading to more interpretable directions than $\mathcal{L}^{cur}$. b) In case $\mathcal{L}^{fso}$ is taken into account, the use of $\mathcal{L}^{cur}$ can significantly improve interpretability compared to $\mathcal{L}^{uur}$ ($\mathcal{S}^1$ in VGG-16 and

Table 19: Ablation study of the method with respect to Uncertainty Region Alignment Losses $\mathcal{L}^{uur}, \mathcal{L}^{cur}$ and the use of Filter-Signal Orthogonality Loss $\mathcal{L}^{fso}$. The network here is EfficientNet trained on ImageNet.

EfficientNet / ImageNet														
I	$\mathcal{L}^{uur}$	$\mathcal{L}^{cur}$	$\mathcal{L}^{fso}$	Coverage ↑	Redundancy ↓	Precision ↑	Recall ↑	F1 ↑	AP ↑	$\mathcal{M}$ ↓	$\mathcal{S}^1$ ↑	$\mathcal{S}^2$ ↑	mIoU ↑	$\mathcal{I}^1$ ↑
960	✓	✗	✗	**0.85**	1.51	**0.75±0.22**	**0.2±0.17**	**0.27±0.17**	**0.38±0.16**	**6.74**	**27.92**	**14.71**	**0.03**	**0.94**
	✗	✓	✗	**0.85**	**1.48**	0.74±0.22	**0.2±0.18**	**0.27±0.17**	0.37±0.16	**6.74**	26.5	14.57	**0.03**	**0.94**
	✓	✗	✓	**0.85**	1.49	0.74±0.23	**0.2±0.18**	**0.27±0.17**	**0.38±0.17**	6.76	26.74	14.58	**0.03**	**0.94**
	✗	✓	✓	**0.85**	**1.48**	0.72±0.23	**0.2±0.18**	**0.27±0.17**	**0.38±0.17**	6.75	25.92	14.45	**0.03**	**0.94**
1120	✓	✗	✗	**0.85**	1.61	**0.76±0.21**	**0.2±0.17**	**0.28±0.17**	**0.39±0.17**	6.73	**31.36**	**16.54**	**0.03**	**0.94**
	✗	✓	✗	**0.85**	1.56	**0.76±0.21**	**0.2±0.18**	**0.28±0.17**	0.38±0.17	**6.72**	29.79	16.39	**0.03**	0.93
	✓	✗	✓	**0.85**	1.56	0.74±0.22	**0.2±0.18**	**0.28±0.18**	**0.39±0.17**	6.76	29.54	16.48	**0.03**	**0.94**
	✗	✓	✓	**0.85**	**1.54**	0.74±0.22	**0.2±0.18**	**0.28±0.19**	**0.39±0.17**	6.74	28.62	16.38	**0.03**	**0.94**
1280	✓	✗	✗	**0.85**	1.65	**0.74±0.21**	**0.19±0.16**	**0.27±0.16**	**0.36±0.17**	6.81	**40.38**	**19.12**	**0.03**	**0.94**
	✗	✓	✗	**0.85**	1.67	**0.74±0.21**	**0.19±0.17**	**0.27±0.17**	**0.36±0.17**	**6.8**	36.5	18.67	**0.03**	0.93
	✓	✗	✓	**0.85**	1.63	0.73±0.2	**0.19±0.17**	0.26±0.17	**0.36±0.17**	6.9	37.67	18.96	**0.03**	**0.94**
	✗	✓	✓	**0.85**	**1.6**	0.73±0.21	**0.19±0.17**	0.26±0.17	**0.36±0.17**	6.88	36.95	18.98	**0.03**	**0.94**

Table 20: Ablation study of the method with respect to Uncertainty Region Alignment Losses $\mathcal{L}^{uur}, \mathcal{L}^{cur}$ and the use of Filter-Signal Orthogonality Loss $\mathcal{L}^{fso}$. The network here is Inception-v3 trained on ImageNet.

Inception-v3 / ImageNet														
I	$\mathcal{L}^{uur}$	$\mathcal{L}^{cur}$	$\mathcal{L}^{fso}$	Coverage ↑	Redundancy ↓	Precision ↑	Recall ↑	F1 ↑	AP ↑	$\mathcal{M}$ ↓	$\mathcal{S}^1$ ↑	$\mathcal{S}^2$ ↑	mIoU ↑	$\mathcal{I}^1$ ↑
1536	✓	✗	✗	**0.87**	2.41	0.84±0.18	0.28±0.24	0.38±0.26	0.53±0.26	**6.79**	**156.46**	**28.03**	**0.11**	0.93
	✗	✓	✗	0.85	2.09	0.85±0.19	**0.3±0.23**	**0.4±0.25**	0.56±0.25	6.86	156.42	27.88	**0.11**	0.93
	✓	✗	✓	0.85	1.94	0.85±0.21	0.22±0.16	0.33±0.19	0.57±0.24	6.88	123.85	27.08	0.08	**0.94**
	✗	✓	✓	0.85	**1.9**	**0.86±0.19**	0.23±0.16	0.33±0.19	**0.58±0.24**	6.87	125.64	27.46	0.08	**0.94**
1792	✓	✗	✗	**0.9**	2.96	0.86±0.16	**0.33±0.25**	0.43±0.26	0.58±0.25	**6.77**	**210.44**	**25.77**	**0.13**	0.93
	✗	✓	✗	0.85	2.45	0.88±0.16	**0.33±0.25**	**0.44±0.26**	**0.59±0.24**	6.84	208.6	24.98	0.12	0.93
	✓	✗	✓	0.87	2.23	**0.89±0.16**	0.24±0.16	0.35±0.19	0.62±0.21	6.89	173.17	24.93	0.1	**0.94**
	✗	✓	✓	0.86	**2.19**	**0.89±0.16**	0.24±0.16	0.36±0.19	0.62±0.21	6.92	174.0	24.69	0.1	**0.94**
2048	✓	✗	✗	0.86	**2.36**	**0.85±0.2**	**0.31±0.29**	**0.4±0.29**	**0.54±0.28**	6.95	**170.81**	**32.13**	**0.09**	**0.94**
	✗	✓	✗	0.9	4.85	0.77±0.18	0.3±0.27	0.39±0.27	0.48±0.26	**6.91**	165.65	30.12	0.08	**0.94**
	✓	✗	✓	0.92	4.0	0.75±0.18	0.16±0.12	0.24±0.14	0.38±0.16	7.09	92.53	31.14	0.05	**0.94**
	✗	✓	✓	**0.93**	3.98	0.75±0.18	0.16±0.12	0.24±0.14	0.38±0.16	7.09	92.67	31.18	0.05	**0.94**

ResNet50) or remain comparable to $\mathcal{L}^{uur}$ (ResNet18, EfficientNet, and Inception-v3). c) When comparing among the same type of Uncertainty Region Alignment with and without $\mathcal{L}^{fso}$, in most cases, the use of $\mathcal{L}^{fso}$ hurts interpretability (especially F1-Score and $\mathcal{S}^1$) with the latter being more prominent in Inception-v3 ($I = 2048$) and all cluster sizes of VGG-16 and ResNet50. An interesting exception is that the use of $\mathcal{L}^{fso}$ improves cluster diversity ($\mathcal{S}^2$) in ResNet50. d) Under the same $\mathcal{L}^{fso}$ setting, using $\mathcal{L}^{cur}$ leads to directions with greater significant influence (SDC & SCDP metrics) compared to $\mathcal{L}^{uur}$, except for when using $\mathcal{L}^{fso}$ in ResNet50. e) When considering the same Uncertainty Region Alignment loss variant, the use of $\mathcal{L}^{fso}$ leads to an improvement in the SDC and SCDP metrics, with a notable exception being when using $\mathcal{L}^{cur}$ in ResNet18.

Table 21: Ablation study of the method with respect to Uncertainty Region Alignment Losses $\mathcal{L}^{uur}, \mathcal{L}^{cur}$ and the use of Filter-Signal Orthogonality Loss $\mathcal{L}^{fso}$. The network here is VGG16 trained on ImageNet.

VGG16 / ImageNet														
I	$\mathcal{L}^{uur}$	$\mathcal{L}^{cur}$	$\mathcal{L}^{fso}$	Coverage ↑	Redundancy ↓	Precision ↑	Recall ↑	F1 ↑	AP ↑	$\mathcal{M}$ ↓	$\mathcal{S}^1$ ↑	$\mathcal{S}^2$ ↑	mIoU ↑	$\mathcal{I}^1$ ↑
384	✓	✗	✗	**0.82**	1.17	0.61±0.18	**0.18±0.09**	**0.27±0.09**	**0.31±0.12**	6.88	**29.98**	**9.39**	**0.08**	**0.91**
	✗	✓	✗	0.8	1.09	0.62±0.17	0.17±0.09	0.26±0.09	**0.31±0.11**	**6.87**	28.12	9.09	0.07	0.9
	✓	✗	✓	0.79	**1.05**	0.6±0.17	0.16±0.09	0.24±0.09	**0.31±0.11**	7.12	23.42	8.51	0.06	0.9
	✗	✓	✓	0.79	1.07	**0.63±0.18**	0.16±0.09	0.24±0.09	**0.31±0.12**	6.92	26.23	8.89	0.07	0.9
448	✓	✗	✗	**0.84**	1.35	0.59±0.18	**0.18±0.09**	**0.26±0.09**	**0.3±0.11**	6.93	**34.67**	**10.29**	**0.08**	**0.91**
	✗	✓	✗	0.82	1.22	0.6±0.18	0.17±0.08	0.25±0.09	**0.3±0.11**	**6.92**	32.18	9.53	0.07	0.9
	✓	✗	✓	0.82	**1.18**	0.58±0.17	0.15±0.08	0.23±0.09	**0.3±0.11**	7.14	26.72	8.75	0.06	0.9
	✗	✓	✓	0.82	1.22	**0.61±0.18**	0.16±0.08	0.24±0.09	**0.3±0.11**	6.93	30.91	9.26	0.07	0.9
512	✓	✗	✗	**0.85**	1.43	0.61±0.18	**0.18±0.08**	**0.27±0.09**	**0.31±0.11**	**6.95**	**41.2**	**11.11**	**0.08**	**0.91**
	✗	✓	✗	**0.85**	1.39	**0.62±0.17**	**0.18±0.08**	0.26±0.09	0.3±0.11	6.96	39.23	10.88	**0.08**	0.9
	✓	✗	✓	**0.85**	**1.35**	0.59±0.18	0.15±0.09	0.22±0.09	0.29±0.11	7.23	28.62	10.4	0.06	0.9
	✗	✓	✓	**0.85**	1.37	**0.62±0.18**	0.15±0.09	0.24±0.09	0.3±0.11	7.09	33.91	10.83	0.07	0.9

Table 22: Ablation study of the method with respect to Uncertainty Region Alignment Losses $\mathcal{L}^{uur}, \mathcal{L}^{cur}$ and the use of Filter-Signal Orthogonality Loss $\mathcal{L}^{fso}$. The network here is ResNet50 trained on Moments in Time.

ResNet50 / MiT														
I	$\mathcal{L}^{uur}$	$\mathcal{L}^{cur}$	$\mathcal{L}^{fso}$	Coverage ↑	Redundancy ↓	Precision ↑	Recall ↑	F1 ↑	AP ↑	$\mathcal{M}$ ↓	$\mathcal{S}^1$ ↑	$\mathcal{S}^2$ ↑	mIoU ↑	$\mathcal{I}^1$ ↑
1536	✓	✗	✗	0.84	**2.13**	0.72±0.22	**0.17±0.12**	**0.26±0.15**	0.36±0.16	**6.25**	127.83	33.67	0.08	**0.85**
	✗	✓	✗	0.83	2.33	**0.75±0.16**	**0.17±0.12**	**0.26±0.15**	0.35±0.15	**6.25**	**141.4**	30.12	**0.09**	**0.85**
	✓	✗	✓	**0.88**	2.39	0.74±0.19	**0.17±0.12**	0.25±0.14	0.44±0.14	6.59	94.24	**35.05**	0.06	0.84
	✗	✓	✓	**0.88**	2.37	**0.75±0.19**	**0.17±0.11**	**0.26±0.13**	**0.45±0.14**	6.49	98.52	34.81	0.06	0.84
1792	✓	✗	✗	0.85	**2.47**	**0.78±0.16**	**0.19±0.10**	**0.29±0.13**	0.4±0.14	**6.24**	162.86	34.17	**0.09**	**0.85**
	✗	✓	✗	0.83	2.61	0.76±0.16	**0.19±0.11**	**0.29±0.14**	0.38±0.15	6.27	**164.82**	30.63	**0.09**	**0.85**
	✓	✗	✓	**0.89**	2.66	0.75±0.17	0.16±0.11	0.25±0.13	0.43±0.13	6.55	109.36	36.48	0.06	0.84
	✗	✓	✓	0.88	2.62	0.76±0.16	0.16±0.11	0.25±0.13	**0.44±0.13**	6.5	113.9	**36.68**	0.06	0.84
2048	✓	✗	✗	0.86	3.15	0.72±0.2	**0.21±0.13**	**0.31±0.16**	**0.43±0.16**	**6.29**	**209.2**	33.04	**0.1**	**0.85**
	✗	✓	✗	0.83	**2.7**	**0.76±0.15**	0.2±0.11	0.3±0.14	0.42±0.15	6.36	205.22	32.78	**0.1**	**0.85**
	✓	✗	✓	**0.89**	2.9	0.72±0.16	0.15±0.11	0.23±0.12	0.41±0.13	6.61	120.5	35.09	0.06	0.84
	✗	✓	✓	0.88	2.83	0.72±0.16	0.15±0.11	0.24±0.12	**0.43±0.13**	6.61	126.46	**35.98**	0.06	0.84

Table 23: Ablation study of the method with respect to Uncertainty Region Alignment Losses $\mathcal{L}^{uur}, \mathcal{L}^{cur}$ and the use of Filter-Signal Orthogonality Loss $\mathcal{L}^{fso}$. The Table depicts metrics of statistical significant influence. For ResNet18, $I = 448$, for EfficientNet, $I = 1120$ and for ResNet50, $I = 1792$.

			ResNet18 / Places365		**EfficientNet / ImageNet**		**ResNet50 / MiT**	
$\mathcal{L}^{uur}$	$\mathcal{L}^{cur}$	$\mathcal{L}^{fso}$	SDC	SCDP	SDC	SCDP	SDC	SCDP
✓	✗	✗	264	1565	107	243	393	570
✗	✓	✗	**322**	**2285**	**426**	**714**	**1154**	**2250**
✓	✗	✓	**296**	1786	668	1445	**1676**	**7946**
✗	✓	✓	**296**	**1892**	**673**	**1484**	1353	3913

A.11 Comparison with Unsupervised Interpretable Basis Extraction and Concept-Basis Extraction in Practical Experiments

Table 24: Comparison and Ablation with respect to method enhancements that we propose in this work. $\mathcal{L}^{al}$ stands for Augmented Lagrangian Loss and $\mathcal{L}^{cc}$ refers to the CNN Classifier loss that was proposed in Doumanoglou et al. (2024). Methods below the dashed line correspond to variations that use the contributions we make in this work. Here the network is ResNet18 and $I = 512$.

ResNet18 / Places365							
Method	Ortho	$\mathcal{L}^{al}$	$\mathcal{L}^{cc}$	$\mathcal{L}^{uur}$	$\mathcal{L}^{cur}$	$\mathcal{S}^1$	$\mathcal{S}^2$
UIBE (Doumanoglou et al., 2023)	✓	✗	✗	✗	✗	60.93	28.39
CBE (Doumanoglou et al., 2024)	✓	✗	✓	✗	✗	**69.43**	31.53
CBE /w $\mathcal{L}^{uur}$	✓	✗	✗	✓	✗	67.3	32.16
EDDP-U	✗	✓	✗	✓	✗	52.51	**37.78**
EDDP-C	✗	✓	✗	✗	✓	50.29	36.99

Table 25: Comparison and Ablation with respect to method enhancements that we propose in this work. $\mathcal{L}^{al}$ stands for Augmented Lagrangian Loss and $\mathcal{L}^{cc}$ refers to the CNN Classifier loss that was proposed in Doumanoglou et al. (2024). Methods below the dashed line correspond to variations that use the contributions we make in this work. Here the network is ResNet50 and $I = 2048$.

ResNet50 / MiT							
Method	Ortho	$\mathcal{L}^{al}$	$\mathcal{L}^{cc}$	$\mathcal{L}^{uur}$	$\mathcal{L}^{cur}$	$\mathcal{S}^1$	$\mathcal{S}^2$
UIBE (Doumanoglou et al., 2023)	✓	✗	✗	✗	✗	124.73	18.47
CBE (Doumanoglou et al., 2024)	✓	✗	✓	✗	✗	131.73	26.94
CBE/w $\mathcal{L}^{uur}$	✓	✗	✗	✓	✗	158.76	33.02
EDDP-U	✗	✓	✗	✓	✗	**209.2**	33.04
EDDP-C	✗	✓	✗	✗	✓	126.46	**35.98**

Tables 24 and 25 briefly present comparisons of our work with the previous works that we extend, in terms of interpretability. First, with other aspects of Concept Basis Extraction (CBE) (Doumanoglou et al., 2024) being intact, we assess the efficacy of our Unconstrained Uncertainty Region Alignment loss in improving the interpretability of the clustering, compared to the CNN Classifier Loss $\mathcal{L}^{cc}$ that was proposed previously in Doumanoglou et al. (2024). This case is referred to in the tables as *CBE /w* $\mathcal{L}^{uur}$. We observe that in three out of the four cases, our Uncertainty Region Alignment loss leads to a notable relative improvement, by up to 22.56% in $\mathcal{S}^2$, which indicates a clustering with improved concept diversity. When we additionally take into account the rest of our contributions, and compare EDDP-U with CBE, we find that in the same three out of four cases, interpretability is further improved by up to 58.8% in terms of $\mathcal{S}^1$. Transitioning from CBE to EDDP-C, may lead to further improvements in $\mathcal{S}^2$ by up to 33.5%, yet with a decreased score in terms of $\mathcal{S}^1$.

A.12 More Qualitative Segmentations and Statistics for Evaluating the Interpretability of the Concept Detectors

Figures 29, 30, 31, 32, 33, 34, 37, 38, 39 depict qualitative segmentation results obtained using the concept detectors that were learned with the proposed method for the architectures that we studied in this work. Visualizations are obtained using Bau et al. (2017). We can verify that concept detectors appear to be monosemantic. In some cases, there are more than one concept detector detecting the same concept. However, in most cases, the sets of positively classified samples across detectors are disjoint. Figures 35 and 36 depict qualitative segmentations obtained via NMF and PCA. In some of the depicted examples, it is evident that the identified concepts are less monosemantic. Tables 26, 27, 28 and 29 summarize the statistics obtained by Network Dissection regarding the interpretability of the clusterings considered in this work.

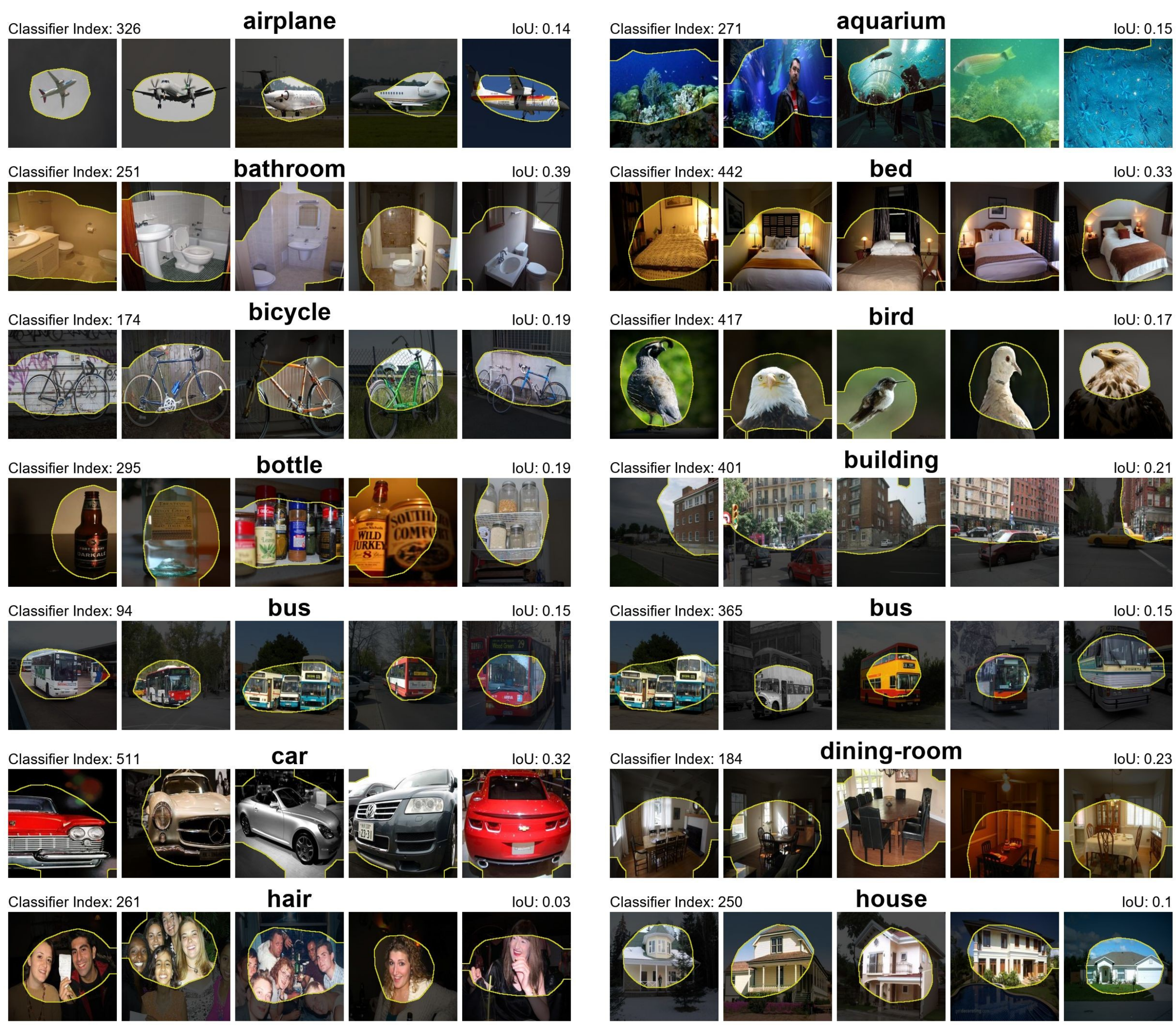


Figure 29: Qualitative segmentations using the concept detectors learned with our method. Here the network is ResNet18 trained on Places365, the method is using CFM, and $I = 512$.

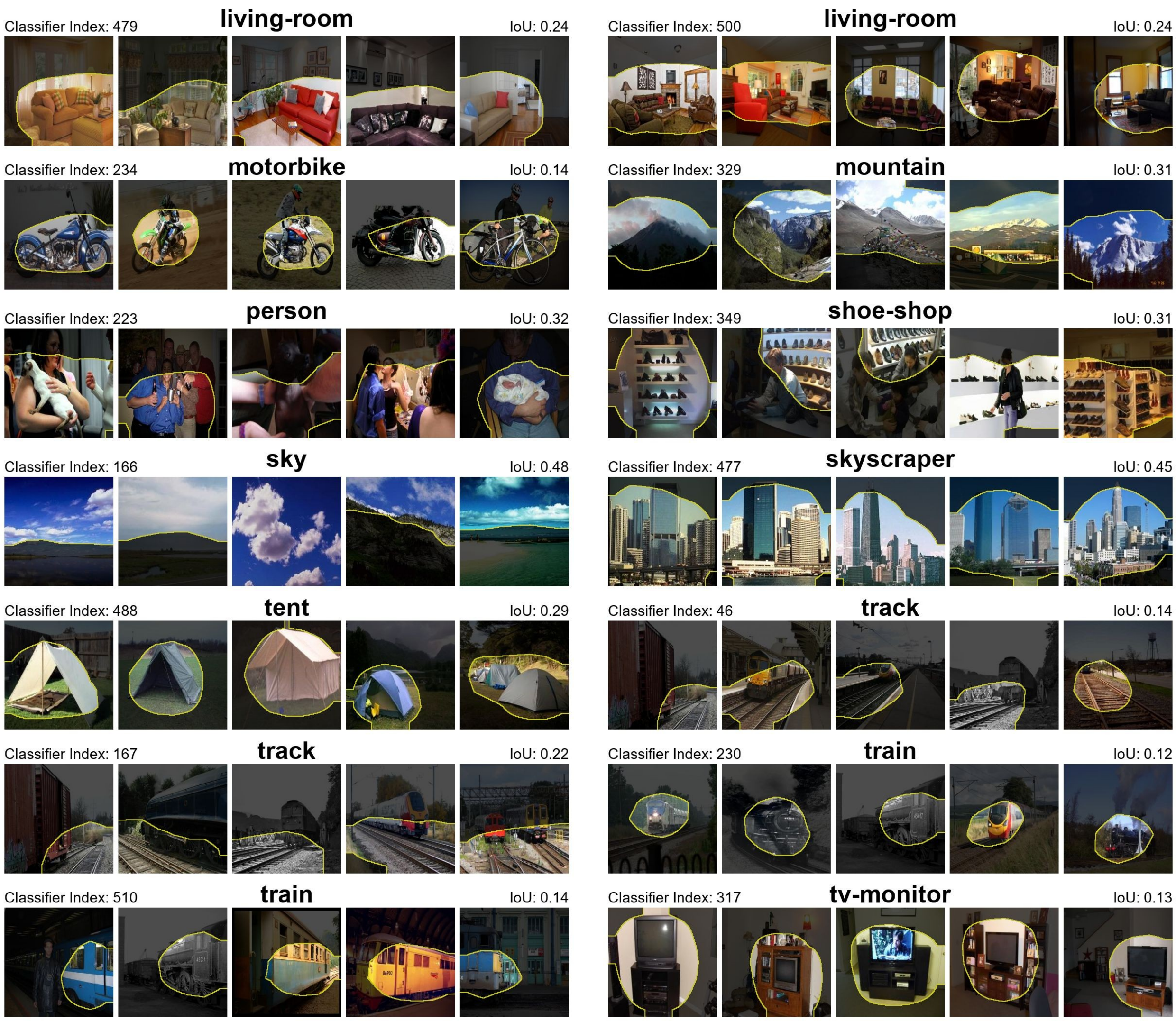


Figure 30: Qualitative segmentations using the concept detectors learned with our method. Here the network is ResNet18 trained on Places365, the method is using CFM, and $I = 512$.

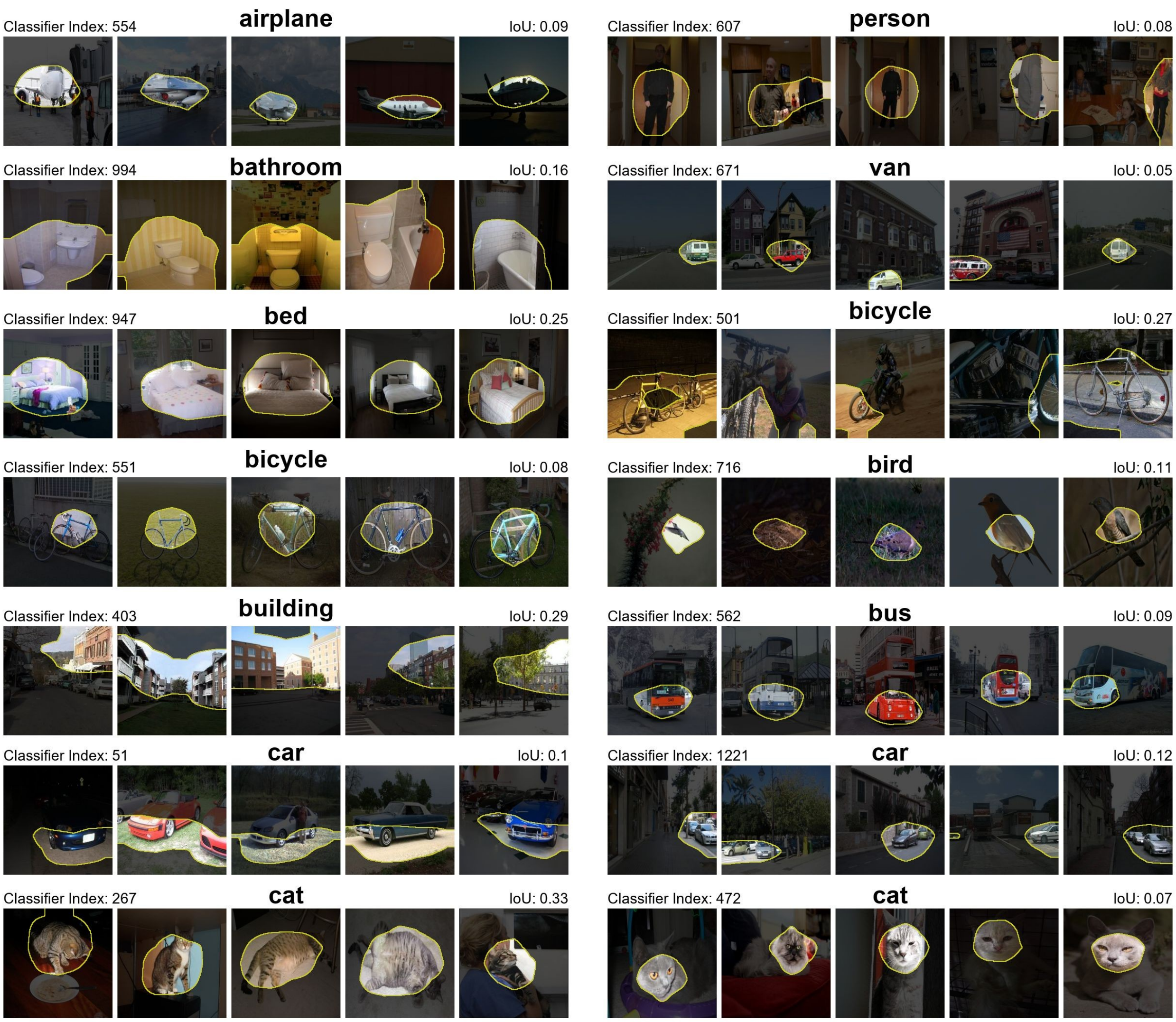


Figure 31: Qualitative segmentations using the concept detectors learned with our method. Here the network is EfficientNet trained on ImageNet, the method is using CFM, and $I = 1280$.

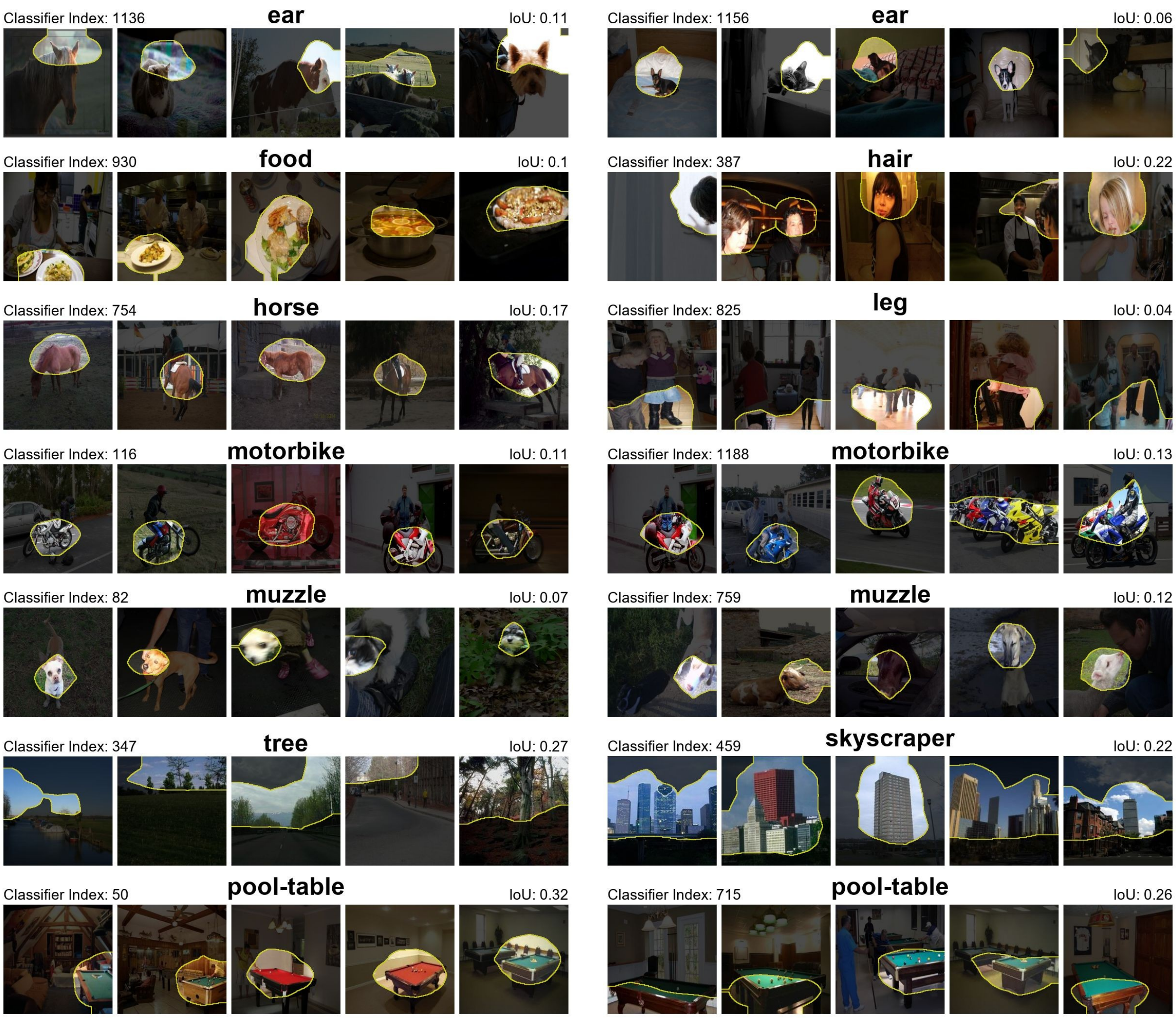


Figure 32: Qualitative segmentations using the concept detectors learned with our method. Here the network is EfficientNet trained on ImageNet, the method is using CFM, and $I = 1280$.

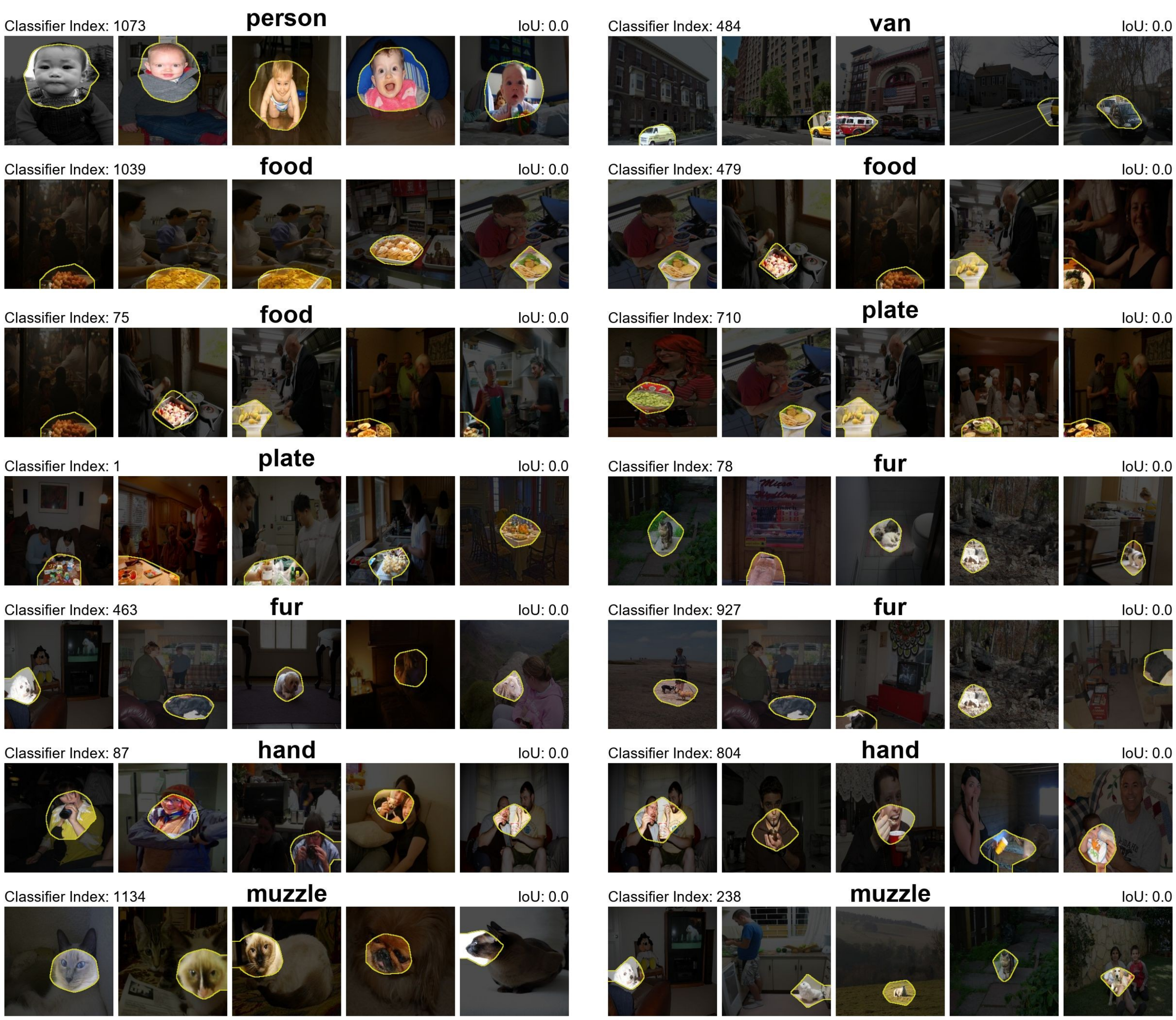


Figure 33: Qualitative segmentations using the concept detectors learned with our method. Here the network is EfficientNet trained on ImageNet, the method is using CFM, and $I = 1280$. All these concept detectors exhibit IoU scores less than 0.04 and Network Dissection does not count them as interpretable. Yet, in many cases these detectors still detect monosemantic concepts.

Figure 34: Qualitative segmentations using the concept detectors learned with our method. Here the network is Inception-v3 trained on ImageNet, the method is using UFM, and $I = 1792$.

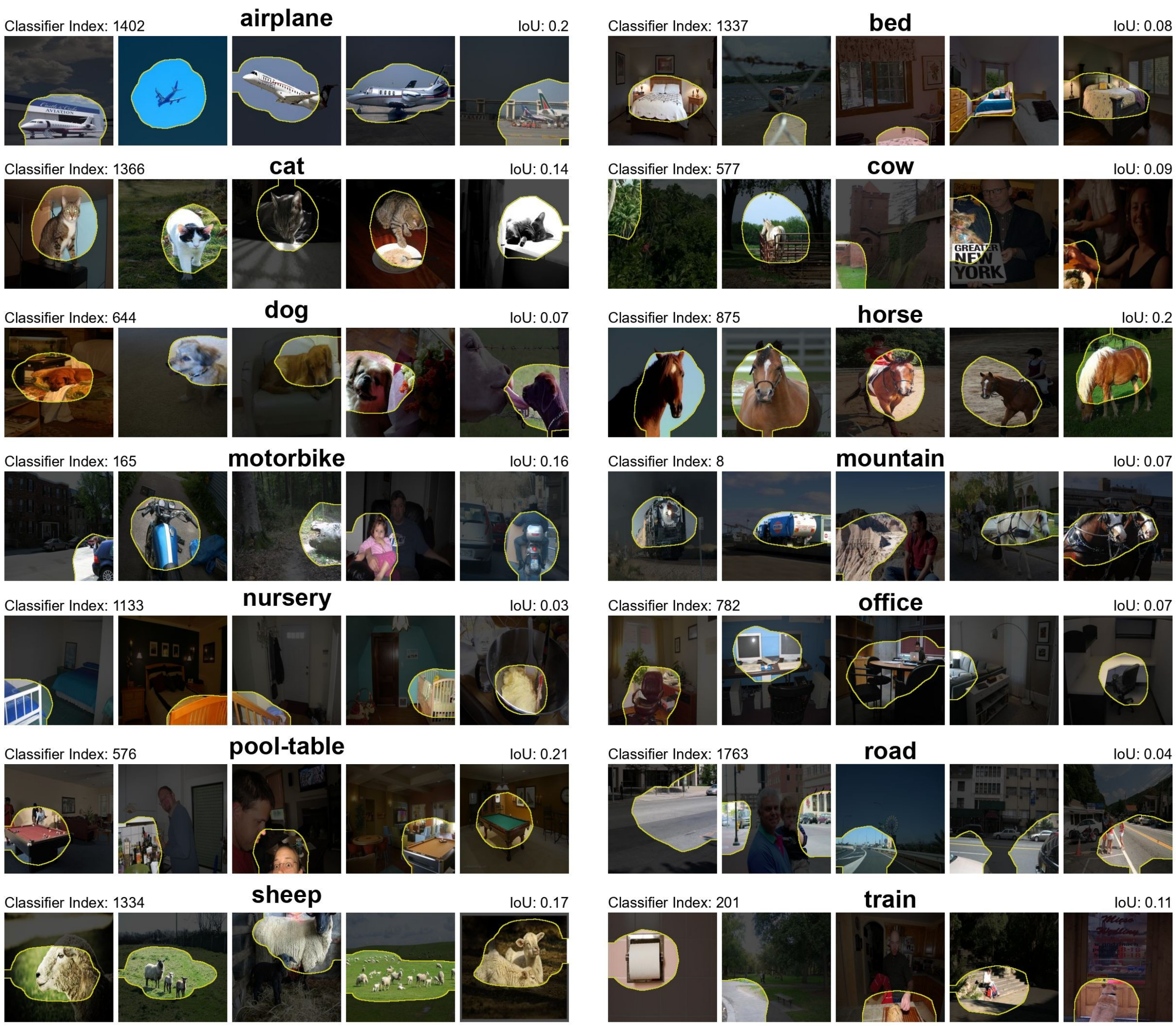


Figure 35: Qualitative segmentations using the factorization of NMF. Here the network is Inception-v3 trained on ImageNet and $I = 1792$.

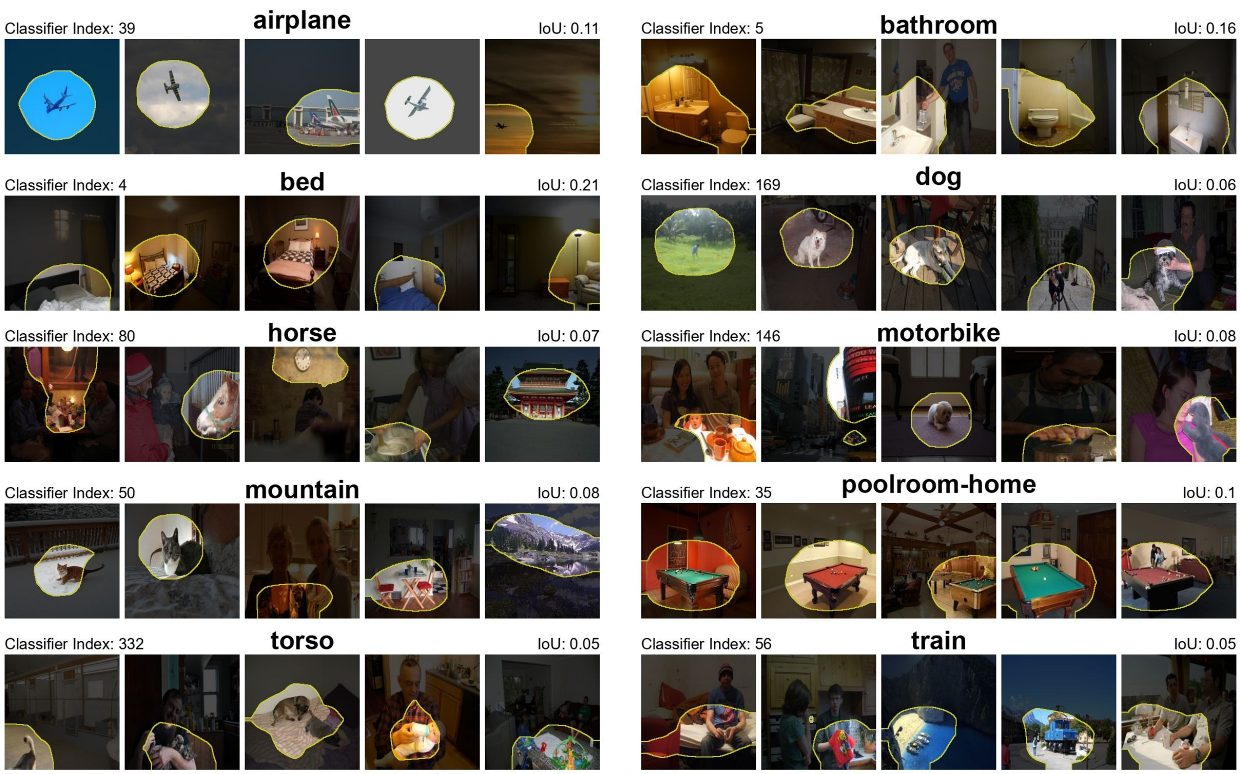


Figure 36: Qualitative segmentations using the concept detectors learned with PCA. Here the network is Inception-v3 trained on ImageNet, and $I = 1792$.

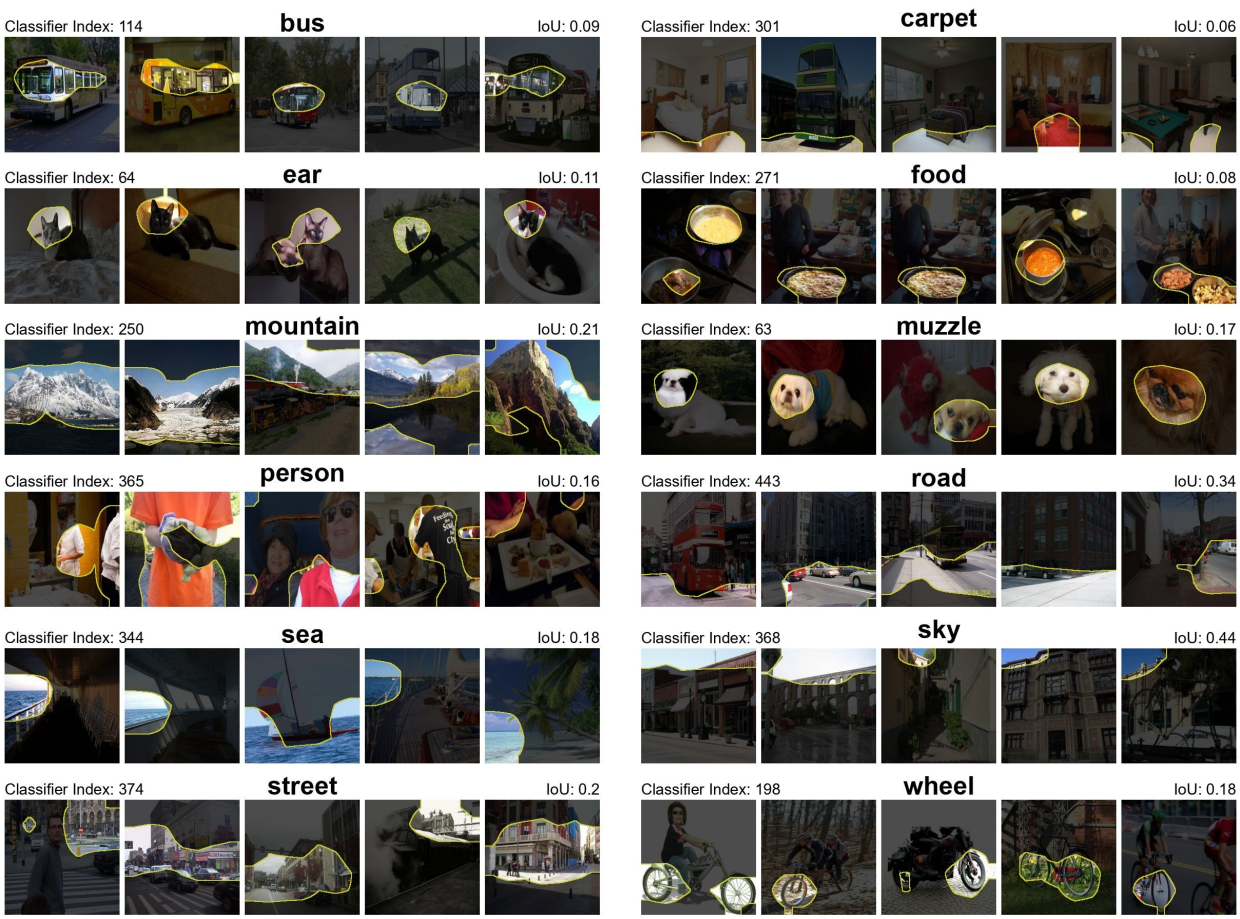


Figure 37: Qualitative segmentations using the concept detectors learned with our method. Here the network is VGG16 trained on ImageNet, the method is using UFM, and $I = 448$.

Figure 38: Qualitative segmentations using the concept detectors learned with our method. Here the network is ResNet50 trained on MiT, the method is using UFM, and $I = 1792$.

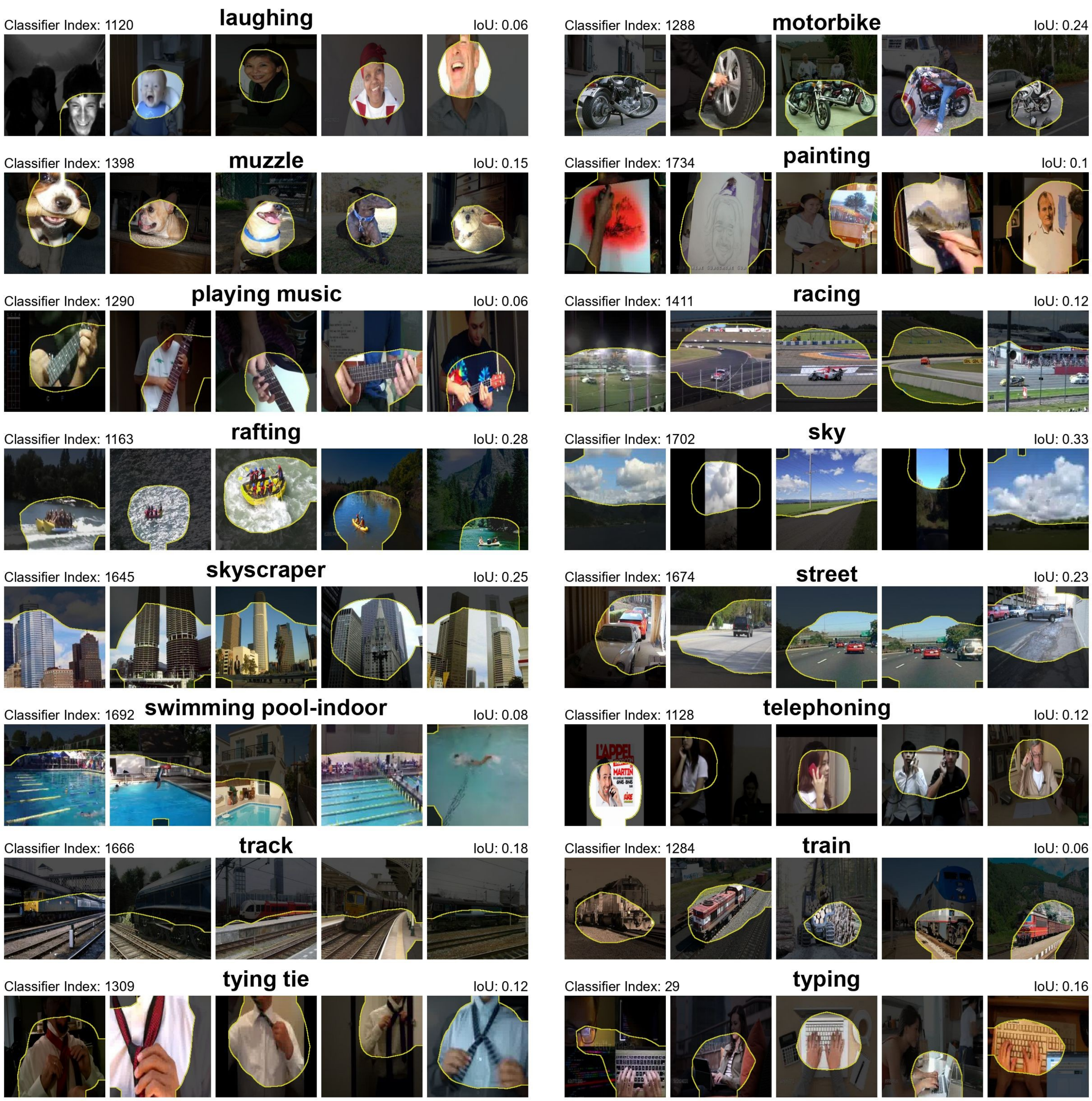


Figure 39: Qualitative segmentations using the concept detectors learned with our method. Here the network is ResNet50 trained on MiT, the method is using UFM, and $I = 1792$.

Table 26: Network Dissection statistics for EfficientNet trained on ImageNet. For each concept category in Broden, we report the two numbers: First, the number of concept detectors that were labeled with the name of a concept belonging to the category and second, the number of unique concept labels from the category that have been assigned to the set of the concept detectors.

			EfficientNet / ImageNet					
I	**Method**	**Color**	**Object**	**Part**	**Material**	**Scene**	**Texture**	**Total**
960	PCA	0 / 0	58 / 15	58 / 4	0 / 0	14 / 5	11 / 4	141 / 28
	EDDP-U	0 / 0	134 / 51	14 / 9	4 / 4	34 / 26	21 / 17	207 / 107
	EDDP-C	0 / 0	120 / 50	13 / 8	5 / 4	35 / 26	21 / 17	194 / 105
1120	PCA	0 / 0	57 / 14	81 / 4	0 / 0	16 / 5	21 / 11	175 / 34
	EDDP-U	0 / 0	137 / 51	26 / 12	5 / 5	39 / 34	18 / 16	225 / 118
	EDDP-C	0 / 0	117 / 52	18 / 9	7 / 5	40 / 35	18 / 16	200 / 117
1280	Natural	0 / 0	155 / 29	28 / 11	1 / 1	29 / 20	10 / 9	223 / 70
	PCA	0 / 0	58 / 15	80 / 4	0 / 0	14 / 5	27 / 14	179 / 38
	EDDP-U	0 / 0	164 / 62	74 / 14	5 / 3	48 / 40	22 / 18	313 / 137
	EDDP-C	0 / 0	132 / 59	60 / 16	6 / 4	47 / 39	22 / 19	267 / 137

Table 27: Network Dissection statistics for Inception-v3 trained on ImageNet. For each concept category in Broden, we report the two numbers: First, the number of concept detectors that were labeled with the name of a concept belonging to the category and second, the number of unique concept labels from the category that have been assigned to the set of the concept detectors.

			Inception-v3 / ImageNet					
I	**Method**	**Color**	**Object**	**Part**	**Material**	**Scene**	**Texture**	**Total**
1536	PCA	0 / 0	58 / 15	60 / 2	0 / 0	18 / 7	155 / 26	291 / 50
	NMF	0 / 0	325 / 44	14 / 5	4 / 2	210 / 58	174 / 42	727 / 151
	EDDP-U	0 / 0	763 / 73	16 / 11	8 / 7	111 / 81	55 / 36	953 / 208
	EDDP-C	0 / 0	593 / 76	16 / 12	7 / 5	104 / 78	47 / 31	767 / 202
1792	PCA	0 / 0	60 / 15	42 / 2	0 / 0	19 / 8	126 / 24	247 / 49
	NMF	0 / 0	340 / 47	14 / 6	2 / 1	207 / 64	137 / 38	700 / 156
	EDDP-U	0 / 0	992 / 65	12 / 7	6 / 5	103 / 76	33 / 27	1146 / 180
	EDDP-C	0 / 0	877 / 67	11 / 10	6 / 5	95 / 72	32 / 28	1021 / 182
2048	Natural	0 / 0	394 / 42	13 / 5	2 / 1	270 / 56	154 / 34	833 / 138
	PCA	0 / 0	57 / 15	58 / 2	0 / 0	19 / 8	153 / 25	287 / 5
	EDDP-U	0 / 0	701 / 85	23 / 15	6 / 5	197 / 113	60 / 38	987 / 256
	EDDP-C	0 / 0	488 / 75	22 / 13	7 / 4	263 / 113	73 / 38	853 / 243

Table 28: Network Dissection statistics for VGG16 trained on ImageNet. For each concept category in Broden, we report the two numbers: First, the number of concept detectors that were labeled with the name of a concept belonging to the category and second, the number of unique concept labels from the category that have been assigned to the set of the concept detectors.

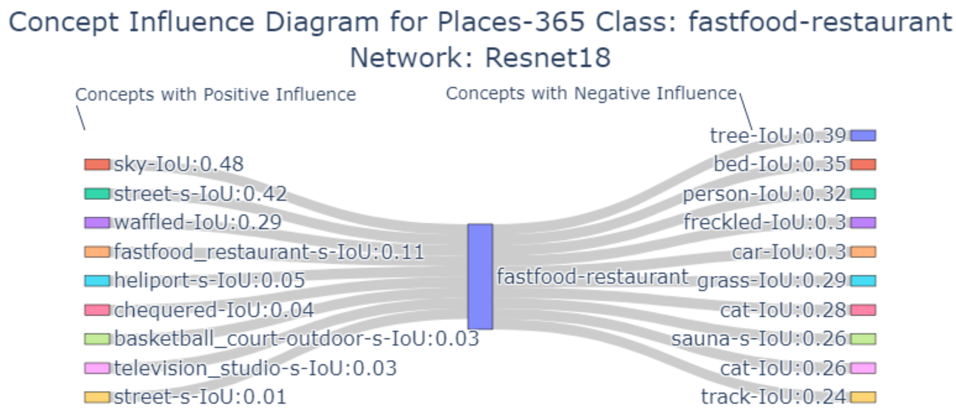
			VGG16 / ImageNet					
I	**Method**	**Color**	**Object**	**Part**	**Material**	**Scene**	**Texture**	**Total**
384	PCA	0 / 0	171 / 11	72 / 5	0 / 0	6 / 3	97 / 13	346 / 32
	NMF	0 / 0	109 / 31	33 / 15	4 / 2	24 / 15	45 / 18	215 / 81
	EDDP-U	1 / 1	51 / 36	203 / 13	1 / 1	4 / 3	20 / 19	280 / 73
	EDDP-C	2 / 2	45 / 33	199 / 12	1 / 1	4 / 3	17 / 16	268 / 67
448	PCA	0 / 0	211 / 11	82 / 5	0 / 0	5 / 3	113 / 15	411 / 34
	NMF	0 / 0	124 / 32	43 / 13	4 / 1	24 / 16	47 / 20	242 / 82
	EDDP-U	0 / 0	63 / 34	237 / 13	5 / 4	10 / 9	18 / 16	333 / 76
	EDDP-C	0 / 0	61 / 35	238 / 12	2 / 1	7 / 6	15 / 13	323 / 67
512	Natural	0 / 0	169 / 34	48 / 14	6 / 2	26 / 17	63 / 23	312 / 90
	PCA	0 / 0	263 / 11	84 / 5	0 / 0	6 / 4	117 / 18	470 / 38
	EDDP-U	1 / 1	71 / 40	267 / 14	2 / 2	11 / 10	25 / 19	377 / 86
	EDDP-C	1 / 1	68 / 40	260 / 14	2 / 2	10 / 9	26 / 19	367 / 85

Table 29: Network Dissection statistics for ResNet50 trained on Moments In Time. For each concept category in Broden, we report the two numbers: First, the number of concept detectors that were labeled with the name of a concept belonging to the category and second, the number of unique concept labels from the category that have been assigned to the set of the concept detectors.

			ResNet50 / MiT						
I	**Method**	**Color**	**Object**	**Part**	**Material**	**Action**	**Scene**	**Texture**	**Total**
1536	PCA	0 / 0	15 / 9	5 / 2	0 / 0	1 / 1	14 / 5	657 / 29	692 / 46
	NMF	0 / 0	214 / 32	18 / 5	0 / 0	279 / 85	109 / 44	308 / 31	928 / 197
	EDDP-U	1 / 1	585 / 54	4 / 4	1 / 1	509 / 134	128 / 60	44 / 31	1272 / 285
	EDDP-C	1 / 1	459 / 54	22 / 5	1 / 1	386 / 143	73 / 58	46 / 30	988 / 292
1792	PCA	0 / 0	17 / 12	5 / 2	0 / 0	1 / 1	13 / 4	683 / 29	719 / 48
	NMF	0 / 0	199 / 35	23 / 5	1 / 1	468 / 111	99 / 46	144 / 22	934 / 220
	EDDP-U	0 / 0	673 / 52	4 / 4	2 / 2	680 / 135	161 / 67	35 / 23	1555 / 283
	EDDP-C	0 / 0	541 / 51	29 / 6	1 / 1	502 / 150	81 / 63	41 / 24	1195 / 295
2048	Natural	0 / 0	282 / 34	20 / 5	1 / 1	348 / 93	121 / 43	362 / 29	1134 / 205
	PCA	0 / 0	16 / 10	5 / 2	0 / 0	1 / 1	13 / 4	730 / 29	765 / 46
	EDDP-U	0 / 0	768 / 45	5 / 5	1 / 1	709 / 109	377 / 75	49 / 30	1909 / 265
	EDDP-C	0 / 0	542 / 49	112 / 5	2 / 2	648 / 136	94 / 66	51 / 31	1449 / 289

A.13 More Global Model Explanations via Concept Sensitivity Testing

This Section complements Section 7.8. Figures 40, 41 and 42 depict Concept Influence Diagrams for classes of ResNet18 trained on Places365. while Figures 43 and 44 depict diagrams for ResNet50 trained on Moments in Time.



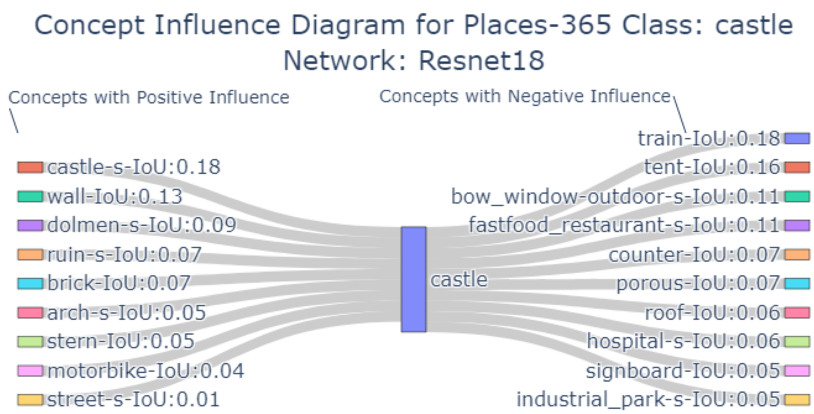
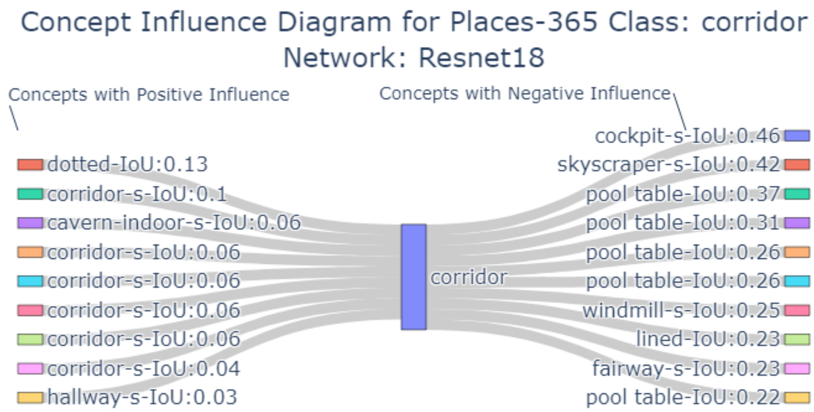


Figure 40: Concept Influence Diagram for ResNet18 trained on Places365. The model is sensitive to the depicted concepts with an absolute score above 0.99. (We use RCAV to quantify the sensitivity, and re-scale the score to $[-1, 1]$) Positive influencing and negative influencing concepts are provided. The number of concepts have been limited to 10. When concepts appear more than once, they correspond to different signal directions (as labeling the classifiers with NetDissect may assign the same concept name to more than one directions.). Here we report results for EDDP-C and $I = 512$.



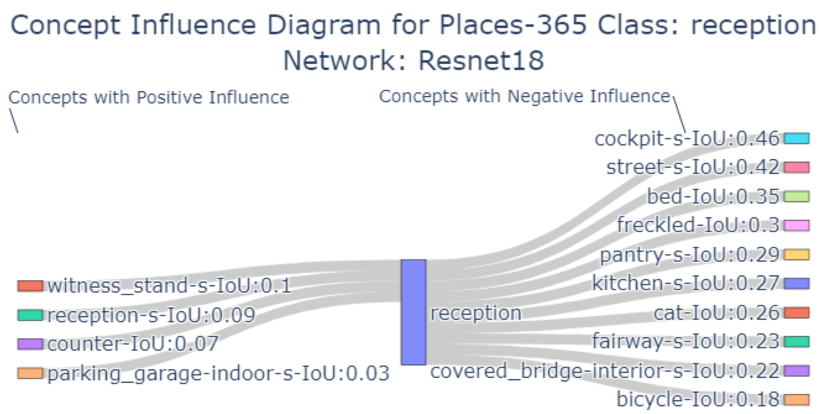
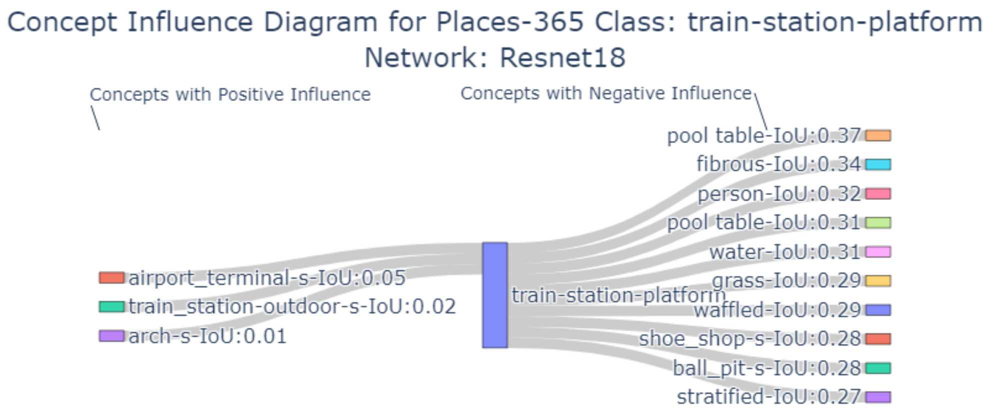


Figure 41: Concept Influence Diagram for ResNet18 trained on Places365. The model is sensitive to the depicted concepts with an absolute score above 0.99. (We use RCAV to quantify the sensitivity, and re-scale the score to $[-1, 1]$) Positive influencing and negative influencing concepts are provided. The number of concepts have been limited to 10. When concepts appear more than once, they correspond to different signal directions (as labeling the classifiers with NetDissect may assign the same concept name to more than one directions.) Here we report results for EDDP-C and $I = 512$.



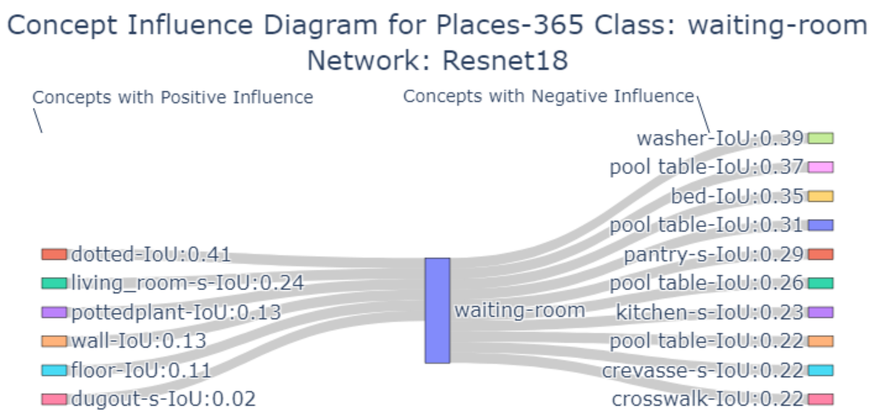
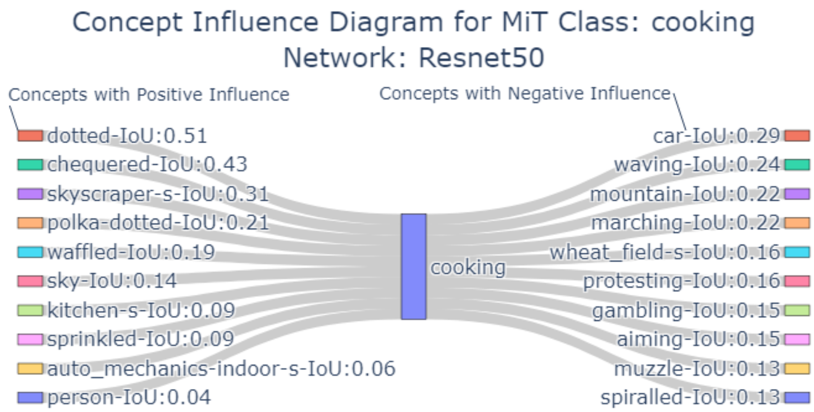


Figure 42: Concept Influence Diagram for ResNet18 trained on Places365. The model is sensitive to the depicted concepts with an absolute score above 0.99. (We use RCAV to quantify the sensitivity, and re-scale the score to $[-1, 1]$) Positive influencing and negative influencing concepts are provided. The number of concepts have been limited to 10. When concepts appear more than once, they correspond to different signal directions (as labeling the classifiers with NetDissect may assign the same concept name to more than one directions.) Here we report results for EDDP-C and $I = 512$.



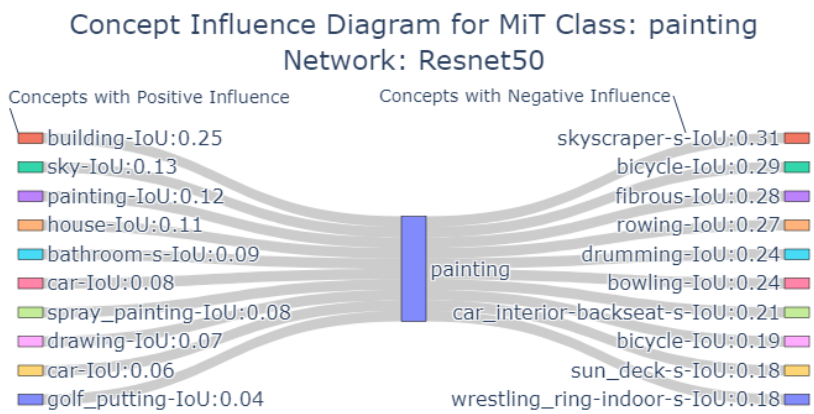
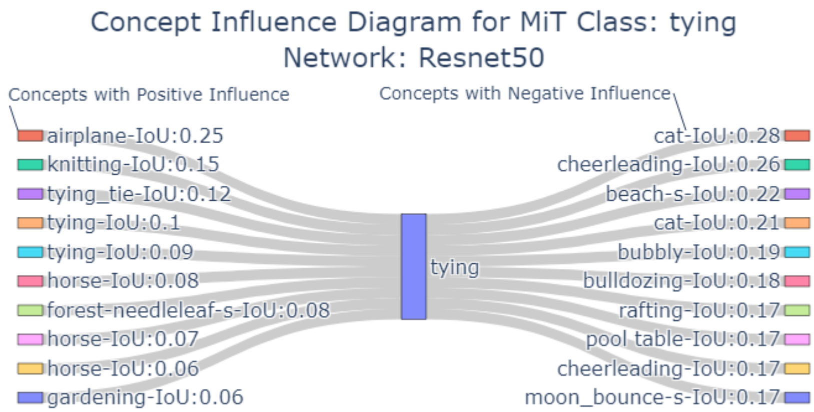


Figure 43: Concept Influence Diagram for ResNet50 trained on Moments in Time (MiT). The model is sensitive to the depicted concepts with an absolute score above 0.99. (We use RCAV to quantify the sensitivity, and re-scale the score to $[-1, 1]$) Positive influencing and negative influencing concepts are provided. The number of concepts have been limited to 10. When concepts appear more than once, they correspond to different signal directions (as labeling the classifiers with NetDissect may assign the same concept name to more than one directions.) Here we report results for EDDP-C and $I = 2048$.



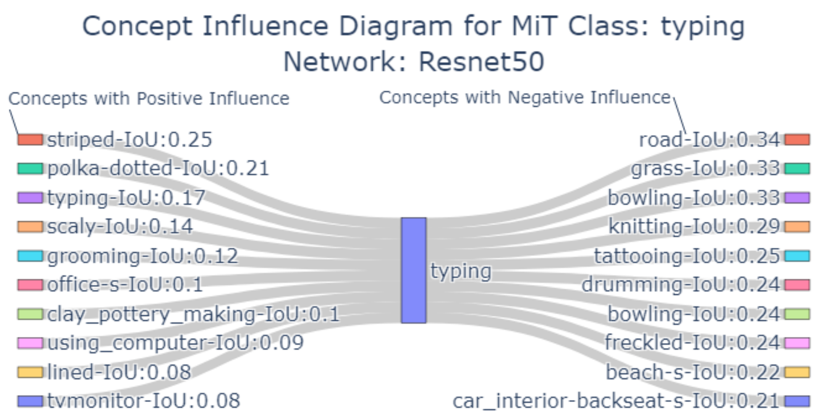


Figure 44: Concept Influence Diagram for ResNet50 trained on Moments in Time (MiT). The model is sensitive to the depicted concepts with an absolute score above 0.99. (We use RCAV to quantify the sensitivity, and re-scale the score to $[-1, 1]$) Positive influencing and negative influencing concepts are provided. The number of concepts have been limited to 10. When concepts appear more than once, they correspond to different signal directions (as labeling the classifiers with NetDissect may assign the same concept name to more than one directions.) Here we report results for EDDP-C and $I = 2048$.

A.14 More Local Explanations with Concept Contribution Maps

This Section complements Section 7.9. Figures 45, 46 depict CCMs for the prediction of an image belonging to class *beach-house*. The respective image concept contribution scores are depicted in Figures 47 and 48. Figures 49, 50 depict CCMs for the prediction of an image belonging to class *bedchamber*. The respective image concept contribution scores are depicted in Figures 51 and 52.

A.15 Relation to Sparse Auto-Encoders

The superposition hypothesis Elhage et al. (2022) assumes that neural networks linearly represent more features than there are neurons in their hidden layers. In this line of work, a feature is defined to be an abstract property of the input, which may or may not align with human intuition, and is exploited by the network to make predictions. Sparse AutoEncoders (SAEs) Bricken et al. (2023) have been proposed as a tool to take features out of superposition; that is, given the activations of a network's intermediate layer, SAEs try to linearly decompose these activations in terms of latent feature components under a sparsity objective.

Let $\boldsymbol{x} \in \mathbb{R}^D$ denote the activation of a network in a hidden layer of study and $I \gg D$ denote the number of latent features that the network is assumed to represent. While several SAE variants have been proposed, such as Lim et al. (2024); Cunningham et al. (2024); Sharkey et al. (2022); Bussmann et al. (2025), in their baseline form Bricken et al. (2023) they first extract latent feature components $\boldsymbol{v}$ by:

$$\boldsymbol{v} = \mathrm{ReLU}(\boldsymbol{W}_{\mathrm{enc}}^T(\boldsymbol{x} - \boldsymbol{b}_{\mathrm{dec}}) + \boldsymbol{b}_{\mathrm{enc}}) \tag{41}$$

and subsequently they aim to reconstruct the original activation by

$$\hat{\boldsymbol{x}} = \boldsymbol{W}_{\mathrm{dec}}\boldsymbol{v} + \boldsymbol{b}_{\mathrm{dec}} \tag{42}$$

with $\boldsymbol{W}_{\mathrm{enc}} \in \mathbb{R}^{D \times I}, \boldsymbol{W}_{\mathrm{dec}} \in \mathbb{R}^{D \times I}, \boldsymbol{b}_{\mathrm{enc}} \in \mathbb{R}^I$ and $\boldsymbol{b}_{\mathrm{dec}} \in \mathbb{R}^D$. The objective that drives SAE learning linearly combines an L2 reconstruction loss between $\boldsymbol{x}$ and $\hat{\boldsymbol{x}}$ and an penalization in the L1 norm of $\boldsymbol{v}$.

To relate SAEs with our approach, we first need to make a correspondence in terms of terminology. First, a SAE *feature*, which is an abstract property of the input, in our terminology is referred to as a *concept*. The *number of latent features* is related to our *concept cluster count*, and we refer to both of them as I. The **encoder** part of the AutoEncoder which is realized by the matrix $\boldsymbol{W}_{\mathrm{enc}}$ is related to our **decoding** directions $\boldsymbol{W}$, while the AutoEncoder's **decoder** part $\boldsymbol{W}_{\mathrm{dec}}$ is equivalent to our **encoding** directions (signal vectors) $\hat{\boldsymbol{S}}$. The SAE's $\boldsymbol{b}_{\mathrm{dec}}$ is related to our multi-concept signal-distractor data model's latent space bias $\boldsymbol{c}$. Finally, a **feature latent** $\boldsymbol{v}$ is somewhat related to the definition of our **signal values**. In particular, under our proposed multi-concept signal-distractor data model, $\boldsymbol{W}_{\mathrm{enc}}^T(\boldsymbol{x} - \boldsymbol{b}_{\mathrm{dec}})$ may be considered as a mechanism to extract signal values.

Despite the conceptual similarities between our method and SAEs, we also have several differences. First, (41) is conceptually acting as a classifier with positive predictions whenever the extracted signal value exceeds the threshold in $\boldsymbol{b}_{\mathrm{enc}}$. From one perspective, the same equation acts like centering the signal value around the classification threshold for the presence of the concept in the representation. In SAEs, sparsity is enforced in the units of the latent features $\boldsymbol{v}$, while in our approach, the ReLU activation function is replaced with a sigmoid, and thus sparsity is enforced in the semantic space of concepts. Second, in SAEs, $\boldsymbol{W}_{\mathrm{dec}}$ are learned via a reconstruction objective, while in our approach, signal vectors are learned under the properties of a probabilistic model constrained on the extracted signal values and the feature activations themselves. Third, we also consider constraining each decoding direction to be perpendicular to the signal vectors of other concepts, for exact signal value extraction. Finally, we also consider uncertainty region alignment which additionally exploits the use of the directions by the model.

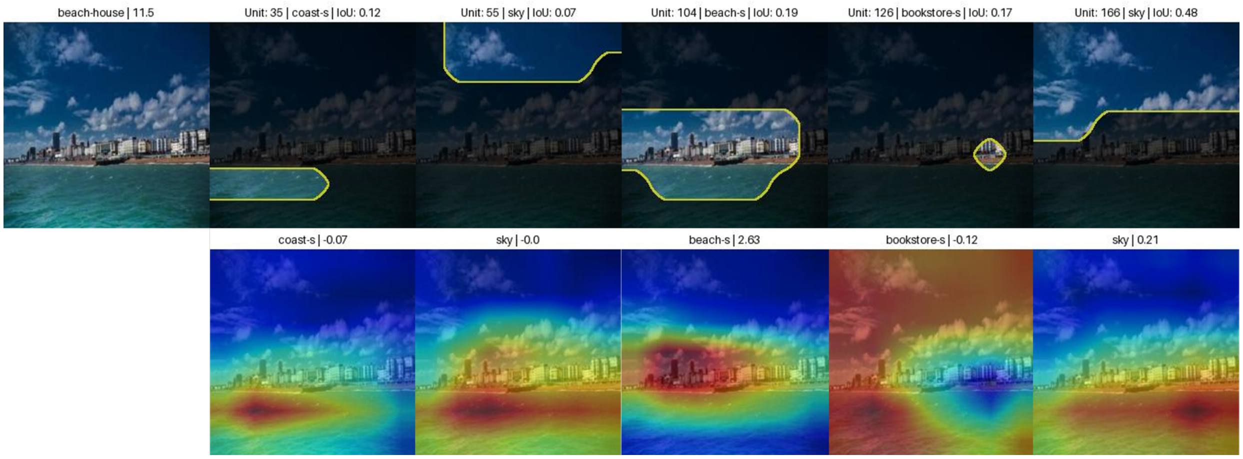


Figure 45: **Left:** Original image. The caption contains class prediction and output class logit. **Top Row:** Segmentation Maps obtained by the concept detectors. The caption contains classifier index (unit), concept-name and IoU score in the validation split of the dataset. **Bottom Row:** Concept Contribution Maps. The caption contains concept-name and contribution of the concept to the class logit.

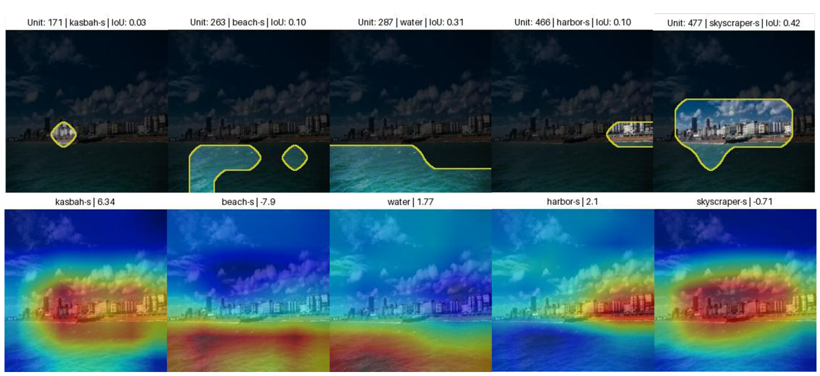


Figure 46: **Top Row:** Segmentation Maps obtained by the concept detectors. The caption contains classifier index (unit), concept-name and IoU score in the validation split of the dataset. **Bottom Row:** Concept Contribution Maps. The caption contains concept-name and contribution of the concept to the class logit.

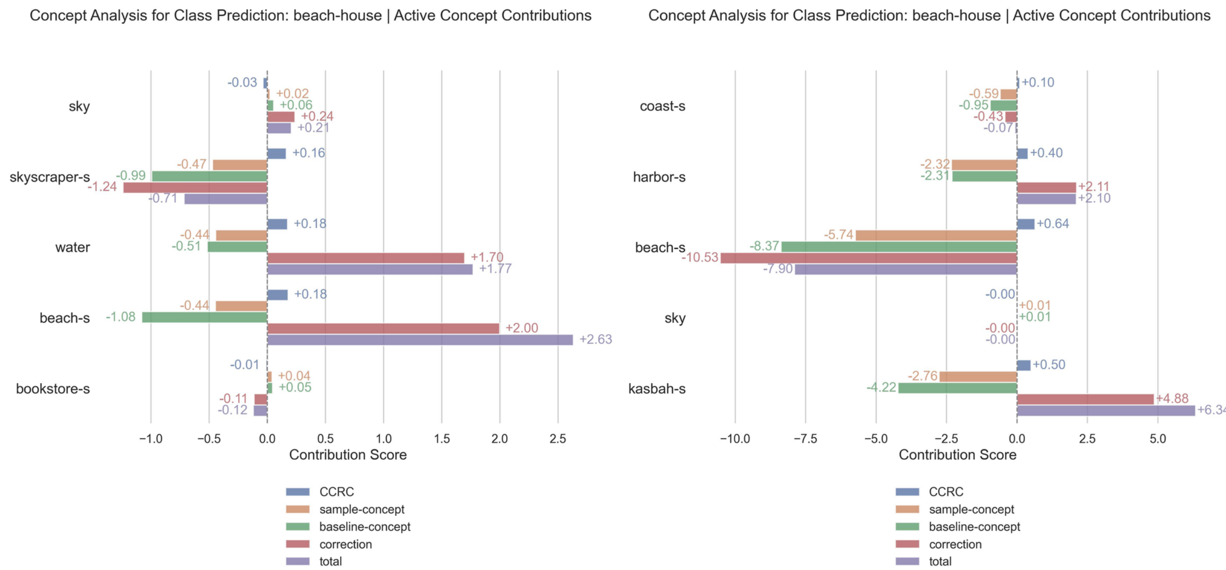


Figure 47: Concept Analysis for predicting an image of the *beach-house* class. The figure depicts concepts found in the image. Even though concepts may share the same name, they correspond to different direction pairs.

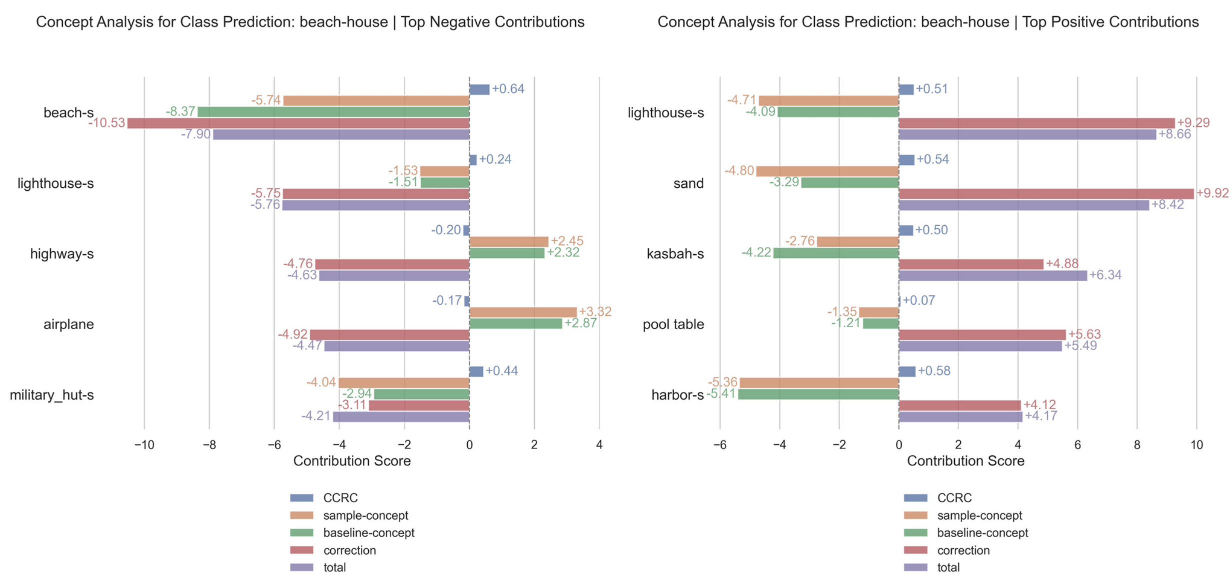


Figure 48: Concept Analysis for predicting an image of the *beach-house* class. The figure depicts top positive and top negative contributing concepts. Even though concepts may share the same name, they correspond to different direction pairs.

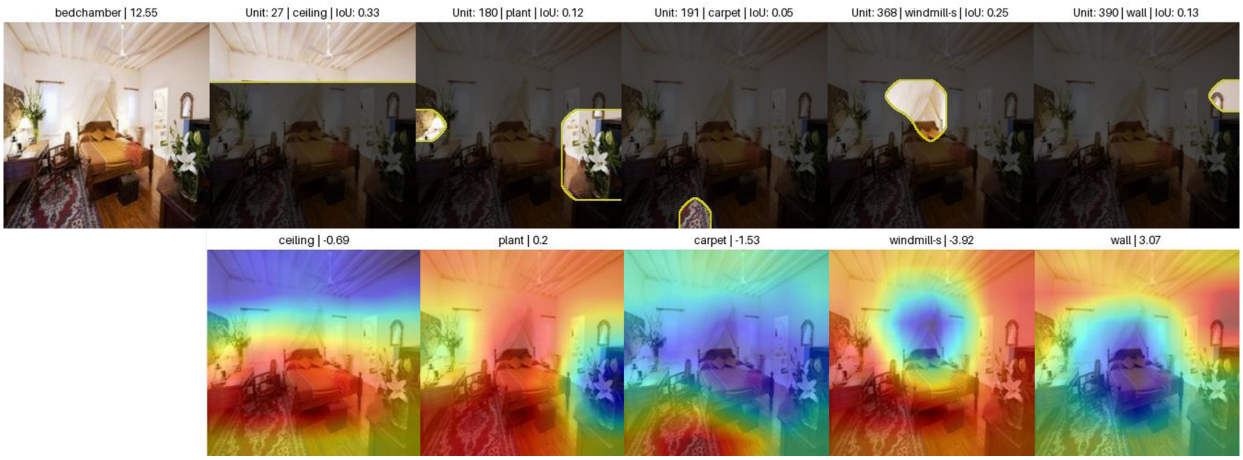


Figure 49: **Left:** Original image. The caption contains class prediction and output class logit. **Top Row:** Segmentation Maps obtained by the Concept Detectors. The caption contains classifier index (unit), concept-name and IoU score in the validation split of the dataset. **Bottom Row:** Concept Contribution Maps. The caption contains concept-name and contribution of the concept to the class logit.

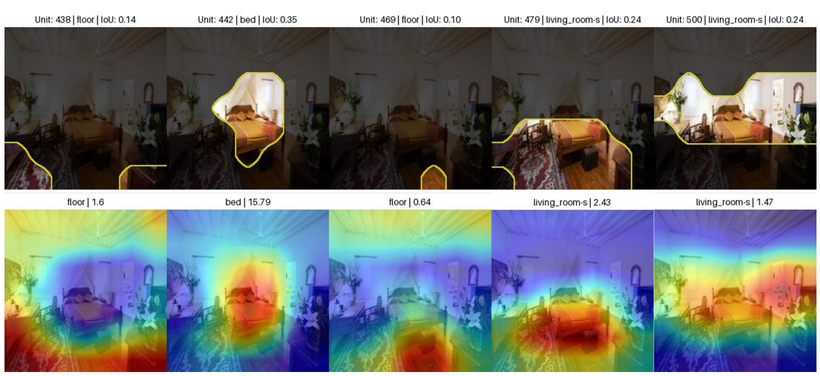


Figure 50: **Top Row:** Segmentation Maps obtained by the concept detectors. The caption contains classifier index (unit), concept-name and IoU score in the validation split of the dataset. **Bottom Row:** Concept Contribution Maps. The caption contains concept-name and contribution of the concept to the class logit.

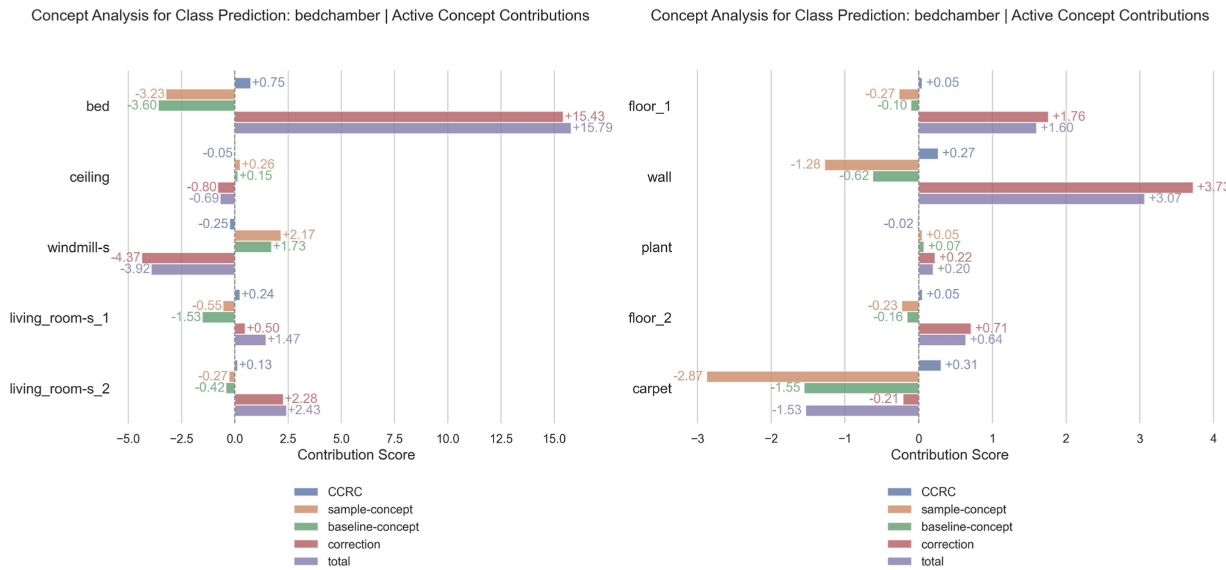


Figure 51: Concept Analysis for predicting an image of the *bedchamber* class. The figure depicts concepts found in the image. Even though concepts may share the same name, they correspond to different direction pairs.

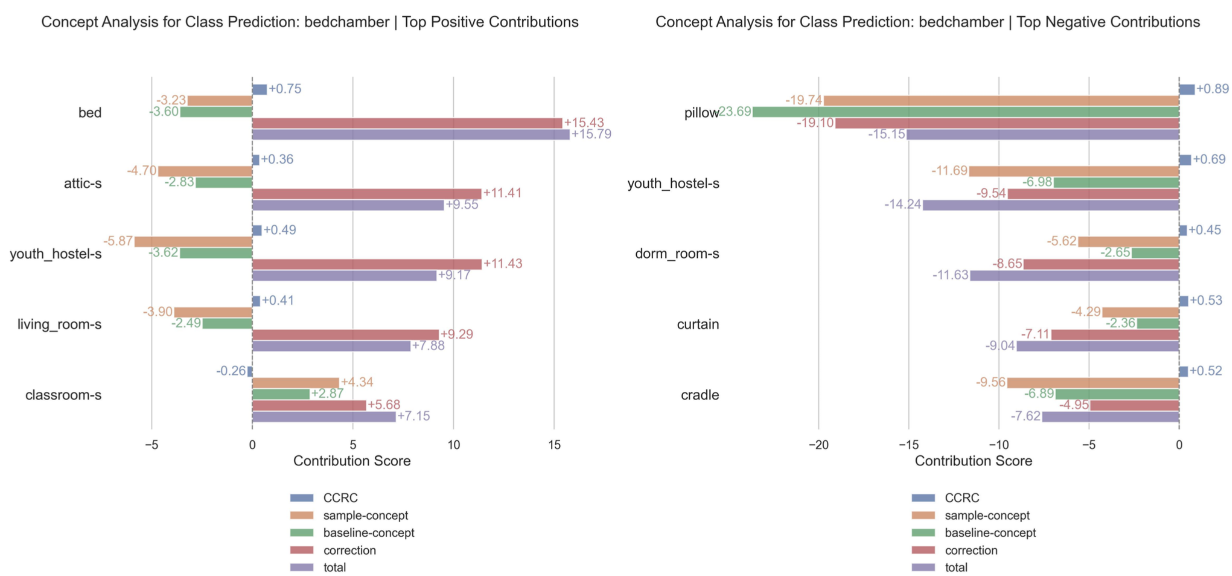


Figure 52: Concept Analysis for predicting an image of the *bedchamber* class. The figure depicts top positive and top negative contributing concepts. Even though concepts may share the same name, they correspond to different direction pairs.