Concept Embedding Analysis: A Review

Gesina Schwalbe (ORCID: 0000-0003-2690-2478)\textsuperscript{1}

\textsuperscript{1}* Continental AG, Regensburg, Germany.

Contributing authors:

gesina.schwalbe@continental-corporation.com;

Abstract

Deep neural networks (DNNs) have found their way into many applications with potential impact on the safety, security, and fairness of human-machine-systems. Such require basic understanding and sufficient trust by the users. This motivated the research field of explainable artificial intelligence (XAI), i.e. finding methods for opening the “black-boxes” DNNs represent. For the computer vision domain in specific, practical assessment of DNNs requires a globally valid association of humanly interpretable concepts with internals of the model. The research field of concept (embedding) analysis (CA) tackles this problem: CA aims to find global, assessable associations of humanly interpretable semantic concepts (e.g., eye, bearded) with internal representations of a DNN. This work establishes a general definition of CA and a taxonomy for CA methods, uniting several ideas from literature. That allows to easy position and compare CA approaches. Guided by the defined notions, the current state-of-the-art research regarding CA methods and interesting applications are reviewed. More than thirty relevant methods are discussed, compared, and categorized. Finally, for practitioners, a survey of fifteen datasets is provided that have been used for supervised concept analysis. Open challenges and research directions are pointed out at the end.

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1 Introduction

Deep neural networks have become a key to many application fields. However, with their popularity, their potential impact to safety and fairness increased to an extend that the need for responsible artificial intelligence (Arrieta et al, 2020) became apparent. For example, the European Union General Data Protection Regulation enacted in 2016 demands algorithms not only to be efficient, but also transparent and fair (Goodman and Flaxman, 2017). Similarly, the automotive functional safety standard ISO 26262 (ISO/TC 22/SC 32, 2018) considers manual inspection of algorithms an important measure of safety assurance. These requirements gave rise to the field of explainable artificial intelligence which was boosted in 2016 by the United States Defense Advanced Research Projects Agency (DARPA) (DARPA, 2016; Adadi and Berrada, 2018). XAI in general tries to translate behavioral or internal aspects of black-box algorithms like DNNs into a human interpretable form (Schwalbe and Finzel, 2021).

While many different aspects of a DNN can be the subject of a human understandable explanation, their safety assessment requires interpretable access to the internal representation. This requirement holds even for hardly specifiable tasks with non-symbolic inputs like object detection from images. This access allows to debug or audit the DNN function with respect to failure modes that violate symbolic prior knowledge (e.g., “eyes usually belong to a movable object”); and this access potentially points out how to fix inappropriate internal representations or directly enforce sufficient ones. Besides the subject of explanation, another relevant property of explainability methods is their locality or scope (Adadi and Berrada, 2018): Many methods for analyzing computer vision DNNs produce local explanations specific to one or few samples (Zhang and Zhu, 2018). In contrast, global explanations are valid for many more examples than would be possible with manual inspection of many local explanations. This makes global explanations interesting for practical assessment tasks. Another practical constraint imposed by assessment use-cases is that explanations must provide high fidelity and that they must be simple (e.g., linear transformations of the object of explanation, as suggested by Kim et al (2018)) to avoid introducing further complexity. Lastly, assessments also require analysis of feature interdependencies and interaction. This is another drawback of solely using the popular heatmapping methods (Zhang et al, 2018b; Janizek et al, 2020) that highlight local attention of a DNN, like relevance (Bach et al, 2015), saliency (Sundararajan et al, 2017), or perturbation (Fong and Vedaldi, 2017) based ones.

A promising class of methods fulfilling the mentioned desires is that of concept (embedding) analysis (CA) methods. The main idea of concept embedding analysis is to associate (in a simple way) semantic concepts taken from natural human language, like eye, with vectors—the concept embedding or concept activation vectors (CAV) (Kim et al, 2018)—, or sub-spaces in the intermediate output space of one (or several) layer(s) in a DNN, the latent space(s). These
approaches allow global access to latent space representations of semantic concepts in an interpretable way, without introducing further complexity. Thus, they fulfill the mentioned desires for assessment tasks and model improvement.

Early work on concept analysis started with unsupervised visualization of single features in convolutional DNNs (CNNs), i.e. neurons, filters or groups thereof (Olah et al, 2017). Later on, supervised approaches were based on the NetDissect method developed in Bau et al (2017), where single filters of CNNs were associated with predefined visual semantic concepts. Two cornerstones towards concept analysis research were established by Fong and Vedaldi (2018) and Kim et al (2018) in 2018. Both methods associate predefined semantic concepts with vectors in the latent spaces, thus post-hoc disentangling the representation of such semantic concepts within DNN internal representations. On this basis, distributed representations in unsupervised settings were first considered in the ACE approach (Ghorbani et al, 2019) proposed in 2019. Another notable development was that of concept bottleneck models (Losch et al, 2019; Koh et al, 2020): Stepping away from post-hoc explainability, these include prior knowledge about task-relevant concepts directly in the architecture of a DNN. This is done with a bottleneck layer in which single nodes are trained to correspond to semantic concepts. These baseline approaches were extended and generalized in many interesting ways in recent years. Thus, time seems to be ready to take a closer look on the developments in this young research area, as will be done in this review.

Contributions

This paper shall shed light onto concept analysis as a practically interesting and emerging sub-field of XAI, in order to foster research in this direction. Its main contributions towards this are as follows:

- A formal, general definition is provided capturing the core ideas uniting concept analysis methods, and differentiating it from similar research fields (cf. Section 3).
- In order to help researchers to find further research directions and position their work, a general taxonomy for concept analysis approaches is developed and applied to state-of-the-art research methods (cf. Section 4 and Figure 1).
- The breadth of the topic is demonstrated by an in-depth and systematic review of more than 30 diverse concept analysis approaches. These are discussed, compared, and categorized according to the taxonomy (cf. Section 4 and Tables 1–4).
- An overview of more than 15 image datasets used for concept analysis is compiled (cf. Section 6 and Table 6).
- Based on the taxonomy and the method reviews, open challenges and promising research directions are uncovered and discussed (cf. Section 7).
4 Concept Embedding Analysis

Scope
This review goes along with the baseline work from Kim et al (2018); Fong and Vedaldi (2018); Bau et al (2017); Ghorbani et al (2019). The main focus lies on visual interpretability, considering computer vision tasks as guiding examples. The literature review combined a two-level recursive reference search starting with the mentioned baselines, and a keyword search based on the keywords “Concept Analysis” and “Concept Embedding Analysis” on the search engine Google Scholar\textsuperscript{1}. Papers were included by a two-stage review approach, first filtering by title and then by the abstract. Included were global interpretability methods that pursue the mentioned general goal of associating human interpretable concepts with DNN latent space vectors or sub-spaces.

Outline
This paper is structured as follows: In Section 2, related work and research fields are recapitulated to demarcate the scope of concept analysis as considered here. A precise definition for concept analysis is then developed in Section 3, and a detailed taxonomy for concept analysis is prescribed. The breadth of the topic is demonstrated in Section 4, in which interesting concept analysis methods are outlined, compared, and classified according to the derived taxonomy (cf. Tables 1–4). Applications of concept analysis are then discussed in Section 5, including model distillation (cf. Table 5) and qualitative as well as quantitative DNN assessment methods. Accompanying these collections, Section 6 compiles an overview on image datasets for supervised concept analysis that are used in methods presented throughout this paper. This may serve as a starting point and reference for researchers looking for typical evaluation datasets. Section 7 provides an outline of current challenges in the area of concept analysis, and an outlook on potential research directions.

2 Related work
The field of XAI has seen an exponential rise in research interest in the last decade (Vilone and Longo, 2020; Arrieta et al, 2020; Linardatos et al, 2021; Zhou et al, 2021). By now, good introductory work is available, like Molnar (2020), and many extensive method surveys, including general ones like Linardatos et al (2021); Vilone and Longo (2020); Arrieta et al (2020); Carvalho et al (2019); Adadi and Berrada (2018); Gilpin et al (2018), and ones specific to sub-topics like reinforcement learning (Heuillet et al, 2021), visual interpretability (Tjoa and Guan, 2020; Zhang and Zhu, 2018), or rule extraction (Hailesilassie, 2016). A meta-review for XAI methods can be found in Schwalbe and Finzel (2021). We also consider the typical XAI method classification aspects of black- versus white-box, post-hoc versus inherent interpretability, and simplicity. These considerations are further refined and tailored to concept analysis in specific, and extended by implementation specific properties of CA methods. A first review on concept analysis is provided

\footnote{https://scholar.google.com/}
by Kazhdan et al (2021), with a two-class scheme for classifying concept analysis methods. In contrast to our broad review, the focus in that work lies on the general practical comparison of two concept analysis approaches with latent space disentanglement. Especially, our review for the first time gives a broad overview of the methods and applications of concept analysis, providing a common point of view of methods usually sorted into very different categories (e.g., post-hoc and inherent interpretability). In the following, related XAI research fields are distinguished from concept analysis.

**Visual attribution methods**

A very popular subfield of XAI is about providing heatmaps that point out what input region (e.g., pixels in an image or words in a text) the DNN mostly attended to make a concrete decision, i.e. which region had the highest attribution. Notable types are perturbation based methods (Ribeiro et al, 2016; Fong and Vedaldi, 2017), relevance back-propagation such as LRP (Bach et al, 2015), activation map based approaches (Zhou et al, 2016), and gradient respectively sensitivity based approaches (Sundararajan et al, 2017). All these approaches find their use in some of the concept analysis applications presented here, e.g., for training (Wu et al, 2020), more precise localization of concepts (Lucieri et al, 2020; Fong and Vedaldi, 2018), or dependency analysis (Kim et al, 2018). While the heatmaps essentially provide a simple linear approximation of the DNN behavior (Ribeiro et al, 2016), these explanations are inherently local and do not provide insights into internal encodings of the DNN. This also prohibits deeper analysis of relations between concepts (Rabold et al, 2020). In contrast, the underlying mapping of concepts to internal features of concept analysis methods is inherently global.

**Latent space disentanglement**

Concept analysis is very closely related to latent space disentanglement (Kazhdan et al, 2021) methods like VAEs (Kingma and Welling, 2014; Higgins et al, 2016), as both approaches try to represent (parts of) the latent space as interpretable features. Similar to so-called concept bottleneck models (Koh et al, 2020), disentanglement methods have a bottleneck layer in which single units are trained to encode a feature. These features, however, are not necessarily aligned with human semantics (especially when trained unsupervised), but instead should encode the most prevalent independent factors of variation causally related to the DNN output. The target features of concept bottleneck models instead are interpretable factors of variation (Kazhdan et al, 2021) perceived by humans. These are not necessarily—and often are not—indepedent, but allow to assess the dependencies of semantic concepts encoded by the DNN.

3 Concept embedding analysis

To get a clear understanding of the scope of concept analysis considered here, related terms are defined in Subsection 3.1, and optional but desirable
properties are collected from literature. Moreover, a taxonomy is provided in Subsection 3.2, that allows a detailed analysis and classification of a use-case or method for CA. The taxonomy is accompanied by illustrative examples, and later applied to the sample methods highlighted in Section 4 (cf. Tables 1–4).

3.1 Definitions

The output of a neural network layer spans a vector space. In this paper, this is called *latent space* of the layer, or *activation maps* if collections of units spatially correspond to patches in the input as in the case of convolutional layers. In this work the term *concept (embedding) analysis* generally refers to investigation of the questions *whether*, *how well*, *how*, and with *which properties* information about a *semantic concept* is represented within the latent spaces or sub-spaces thereof.

*Semantic concepts*

A *(semantic) concept*, also called *attribute* (attr.) in Kronenberger and Haselhoff (2019), is a concept occurring in a natural language, i.e. a notion that can be described using natural language.\(^2\) Examples are the synonym sets established in WordNet (Fellbaum, 1998). The semantic concepts of interest here are those that can be assigned to (patches of) a DNN input sample in the form of additional labels. Hence, the selection of concepts depends on the context given by the task. In Kazhdan et al (2021) this dependency is emphasized in the definition of concepts as interpretable factors of variations for a given training dataset. The paper by Bau et al (2017) introduced the following classes of semantic concepts for images: sample-level attributes like scene (e.g., *rainy*) and image qualities (Abid and Zou, 2021) (e.g., *contrast*); full objects (e.g., *person*); part objects (e.g., *head*, *leg*); and object-level attributes like material (e.g., *wooden*), texture (e.g., *striped*), and color (e.g., *green*). Other examples of object-level attributes are *gender*, and facial attributes like *bearded* as considered in Kim et al (2018). For supervised concept analysis, it is assumed that labeled examples of the concepts of interest are available, and different approaches require different label formats. Formats considered here are the most common binary labels (e.g., Kim et al (2018)) respectively binary segmentation masks (e.g., Fong and Vedaldi (2018); Schwalbe (2021)), multi-class concepts (Kazhdan et al, 2020), and regression concepts (Graziani et al, 2018, 2020). Other possible types are multi-valued concepts with independent values (e.g., *weather* with *raininess* and *cloudiness*), and spatial allocation of concepts, e.g., via bounding boxes or x-y-positions. Note that the direct output of the DNN usually also relates to a semantic concept, like objects for object detectors. The primary interests here are concepts that are not included as features in the DNN final output, e.g., body parts in the case of a pedestrian detector.

\(^2\) Concept terms are marked like this throughout this work.
**Concept analysis (CA)**

By basic concept analysis or concept embedding analysis we define any activity that tries to associate semantic concepts with vectors or sub-spaces in one preselected latent space of a DNN. Further, we assume that this is done via a simple, global model that allows to predict information about the concept from the latent space activations of an input. The model is called the concept model of the concept, and its output depends on the label type of the concept (e.g., binary presence of the concept, localization, regression, classification, etc.). Simple means transparent or human interpretable, or not introducing much more non-interpretable complexity, like linear models (Kim et al, 2018). The pair of a concept and its latent space representation (vector or sub-space) is called the concept embedding. In case a vector is associated, this vector is called the concept vector or concept activation vector (CAV) (Kim et al, 2018).

**Concept analysis goals**

As mentioned previously, the main goals of CA are to answer whether, how well, how, and with which properties information about a predefined or mined semantic concept is represented within a latent space. To just show whether information about a given semantic concept is available within a latent space, one can either perform a supervised training of a concept model and check whether sufficient performance can be reached (Schwalbe, 2021), as illustrated in Fuchs et al (2018); or perform an unsupervised concept mining, later comparing found concept associations with the given concept. A proxy to measure how well the information is encoded generally is the concept model prediction performance. The assessment of properties now requires finding an exact representation of the concept information that can be related or even compared to representations of other concepts (including the input and output). Most common are concept representations by CAVs. The general idea of CAVs is to find a vector which is close to the latent space vectors of examples of the given concept with respect to some proximity measure.

**Desirable properties of concept models**

The following properties of concept models were considered useful in literature:

- **Comparable** concept models allow to assess whether the mapping between semantic and latent space preserves semantic similarities. In other words, whether semantically similar concepts are assigned to similar latent space representations (Schwalbe, 2021).

- **Vector representations** allow to utilize the rich vector space structure of latent spaces, including natural comparability:
  - In Mikolov et al (2013) it was found that for continuous space language models the cosine similarity on latent space vectors correspond to meaningful semantic (cor-)relations of the encoded words. An example is the famous relation “king − man + woman = queen”. Net2Vec (Fong and Vedaldi, 2018) and TCAV (Kim et al, 2018) showed that this also holds for CAVs in computer vision networks,
and Zhang et al (2018b) used cosine similarity for local CAVs modeled by masked derivative vectors.

– The local sensitivity of later layer representations with respect to the concept can easily be measured via the partial derivative along the CAV as proposed in Kim et al (2018).

• **Linear concept models** are considered to be natural and easy to assess for humans in Kim et al (2018).

• **Sparsity** of CAVs in case of linear encodings is postulated to increase interpretability of the concept representations (Bau et al, 2017). Bau et al (2017) even suggest using the number of concepts to which a CNN filter contributes as a comparative measure for interpretability or entanglement—the more filters, the less interpretable.

• Concept models allowing gradient back-propagation, like Net2Vec, can be utilized as additional outputs during training or fine-tuning (Schwalbe and Schels, 2020). Also, they allow to measure attribution of earlier layer concepts or inputs to a given concept output via relevance back-propagation or sensitivity (Lucieri et al, 2020). Otherwise, one has to turn to perturbation-based attribution methods (Wang et al, 2020).

3.2 Taxonomy

In the following we collect key aspects to differentiate approaches for concept embedding analysis, summarized in Figure 1. An overview of how the methods discussed in Section 3 fit into the suggested categorization scheme can be found in Tables 1–4.

**Concept model supervision**

The concepts to be analyzed can either be predefined by sample data and then associated to DNN internal representations in a supervised (superv.) fashion, or human interpretable concepts can be mined from the latent spaces in an unsupervised way. One example of the latter is Automated Concept-based
Explanations (ACE) by Ghorbani et al (2019). They search for clusters in the latent space vectors of super-pixels (the concept candidates), defining a concept by a cluster and the concept vectors as the cluster center. Another example of unsupervised concept analysis is feature visualization (Olah et al, 2017).

**Concept model output: Concept label type**

First concept analysis approaches considered binary concept model outputs, either binary classification (cls) labels as in TCAV (Kim et al, 2018) and ACE, binary segmentation (seg) masks as in Net2Vec (Fong and Vedaldi, 2018), or binary concept center point prediction (det) masks as in Schwalbe and Schels (2020); Rabold et al (2020). This binary setting can be extended to multi-class (mcls) concepts like shape as suggested in Kazhdan et al (2020), or a multi-dimensional concept like in the IIN (Esser et al, 2020) method, where concepts are represented by sub-spaces of the transformed latent space. Regression Concept Vectors (RCV) by Graziani et al (2018), and its successor methods consider continuous-valued instead of discrete-valued concepts.

**Concept model input**

TCAV considers the complete latent space of a layer for its binary classification. The same holds for successor methods that try to mitigate the resulting high memory demand by average pooling of the latent space, like Graziani et al (2020); Chyung et al (2019). However, it is hard to localize concepts in the input only from image level concept information, even using attention methods (Lucieri et al, 2020). To enable localization of concepts, Net2Vec does not consider the complete activation space of a CNN, but instead operates on single pixels of an activation map, utilizing the spatial correspondence between activation map pixels and input regions. In this case of a linear concept model, this can efficiently be implemented by a $1 \times 1$-convolution. The convolutional Net2Vec-approach is adapted in Schwalbe and Schels (2020), only using windows larger than $1 \times 1$ pixels to provide enough context information as input to the concept model. The prior work of Net2Vec on network dissection (Bau et al, 2017) was restricted not only to $1 \times 1$-windows, but also to unit vectors (i.e. single filters) per activation map pixel, similar to standard feature visualization (Olah et al, 2017).

**Concept model type and optimization**

The optimal retrieval of concept information from latent space input can be solved via different models, optimization methods, and regularization constraints. Examples for model types are: small neural networks (e.g., Neural Stethoscopes by Fuchs et al (2018), IIN); k-means clustering (e.g., SeVec by Gu and Tresp (2019), ACE); or more general matrix factorization (e.g., NCAV by Zhang et al (2021); Saini and Papalexakis (2020)); and linear models (e.g., TCAV, Net2Vec). The latter features, e.g., usage of support vector machines (e.g., TCAV), logistic regression (log. regr.) (e.g., Net2Vec, Schwalbe and Schels (2020)), and Bregman iteration (e.g., CHAIN by Wang et al (2020)) for
optimization. It also makes a difference whether a bias is allowed in the linear model or not. Examples of regularization constraints are: Sparsity, as aimed for in NetDissect (Bau et al, 2017), and in CHAIN via $L_1$ loss; and robustness against noise as implemented in Net2Vec and NetDissect by thresholding activation maps.

**Enforcement or post-hoc**

As for other XAI methods, CA approaches can also be classified into inherent interpretability methods enforcing a level of transparency, and post-hoc methods not changing the analyzed DNN like Fong and Vedaldi (2018); Kim et al (2018). Supervised post-hoc CA is called concept localization, and unsupervised post-hoc CA is referred to as concept mining. Typical inherently interpretable architectures utilizing CA are so-called concept-bottleneck models (CBM): These DNNs feature a bottleneck layer in which all or a sub-set of the nodes are trained to be directly associated with a semantic concept. Example architectures and training schemes can be found in Koh et al (2020); Losch et al (2019) (with concept supervision), and ProtoPNet (Chen et al, 2019a) (without concept model output supervision). Different architectures to integrate and connect the concept bottleneck into the DNN are compared in Kronenberger and Haselhoff (2019). Interestingly, good embeddings of task relevant concepts seem to support or at least not decrease the final performance of the network (Losch et al, 2019), and allow for better plausibility checks during operation (Kronenberger and Haselhoff, 2019).

**Comparability: CAV distance measure**

In case concept activation vectors are used to represent concepts in the latent space, both finding and interpreting the vectors often relies on a vector distance measure: For a concept, a CAV is selected which is “close” to latent space vector representations of samples; and to compare concept models based on CAVs, one can also utilize this proximity measure. To our knowledge, three measures have been used in literature:

- **$L_2$ distance** is used for concept mining via clustering in ACE and its successor Yeh et al (2020). It is also used for training a concept localization linear model in the method CHAIN, and the matrix factorization approach NCAV.
- **Cosine similarity** between two vectors $v_1, v_2$ encodes the angle between the vectors and is defined as the normalized dot product
  
  $$\text{CosSim}(v_1, v_2) := \frac{v_1 \circ v_2}{\|v_1\| \cdot \|v_2\|} \in [0, 1]$$

  which is 1 for parallel, 0 for orthogonal, and -1 for anti-parallel vectors. It was used in SeVec (Gu and Tresp, 2019) for concept localization via clustering.
- **Dot product** is the standard distance measure used to define linear models: The model defines a hyperplane $H = \{d_H(v) = v \cdot v_H + b_H = 0\}$ (biased
by $b_H$ where $v_H$ is the normal vector (the concept vector) and $d_H$ defines the signed shortest distance to $H$. This is utilized in the concept localization approaches of TCAV, Net2Vec, and their successors Schwalbe and Schels (2020); Schwalbe (2021), and Kronenberger and Haselhoff (2019).

Other known model types have to use learned distance metrics for comparability.

4 Concept analysis methods

As becomes apparent from the count of taxonomy aspects, there is an abundance of methods to obtain the desired additional concept outputs and concept models inherent to concept analysis. This section deals with prominent example methods to achieve this, and categorizes them according to main aspects of the proposed taxonomy. The first part in Subsection 4.1 discusses methods that work towards inherent transparency and change the underlying model architecture. And the second part in Subsection 4.2 presents methods working on pre-trained models without modifying them, i.e. post-hoc explainability methods. An overview over discussed methods is given in Tables 1–4. Applications for the concept models and outputs will be discussed later in Section 5.

4.1 Inherent concept models

In many applications, inherent interpretability is desirable and may even improve model performance. Examples are safety critical domains like automated driving or medicine, or applications with ethical implications like job application preprocessing. Structuring and training a DNN to use concept embeddings leads to more interpretable intermediate representations respectively models. In the following, it is differentiated between two types of enforcing rich concept outputs: (independent) enforcement of single concepts (Subsubsection 4.1.1), and so-called concept bottleneck models (CBM) enforcing a complete interpretable layer (Subsubsection 4.1.2).

4.1.1 Single concept enforcement

One way to ensure good embeddings of concepts is to add additional outputs for the respective concepts to the DNN and include their predictions into the loss. Such context aware models can be structured like regular DNNs but they use additional regularization to force the network to focus on specific concept embeddings. For example, Schwalbe and Schels (2020) suggested to attach a single neuron per concept (respectively per concept location in the image) and simply add a negative log-likelihood for the prediction performance as weighted summand to the loss.

Neural Stethoscopes. This was implemented in Fuchs et al (2018). They attach 1-hidden-layer DNNs, called Neural Stethoscopes, to the main model which are trained to predict an image-level concept alongside the main output. Their focus was on comparability of the layers, and the Neural Stethoscopes can both be used for concept enforcement and post-hoc concept analysis.
Table 1 Properties of concept analysis methods discussed in Subsubsection 4.1.1 according to the taxonomy defined in Subsection 3.2.

| Method                              | Enforced | Superv. | Model       | Distance measure | Optim. | Label type | Input |
|-------------------------------------|----------|----------|-------------|------------------|--------|------------|-------|
| Single concept enforcement (Subsubsection 4.1.1) | ✓        | ✓        | DNN         | learned log. regr. | cls    | full       |
| Neural Stethoscopes (Fuchs et al, 2018) | ✓        | ✓        | DNN         | learned log. regr. | cls    | full       |
| EDD (Kronenberger and Haselhoff, 2019) | ✓        | ✓        | linear      | dot              | log. regr. | cls    | full       |
| UPerNet (Xiao et al, 2018)           | ✓        | ✓        | DNN         | learned log. regr. | seg    | window     |
| Interpretable CNNs (Zhang et al, 2018c) | ✓        | -        | linear      | dot              | –      | cls        | window |

**EDD.** Similarly, Explanation Dependency Decomposition (EDD) by Kronenberger and Haselhoff (2019) uses additional classifiers to extract the presence of visual embeddings from the convolutional layer outputs. They assessed diverse information flow settings: in-between concept models, and between concept and main model outputs (for details cf. (Kronenberger and Haselhoff, 2019, Fig. 2)). On a simple traffic sign classification setup, adding concept outputs did not infringe performance, and top performance could be achieved by an architecture merging latent space and concept model outputs before predicting the final output.

**UPerNet.** This is extended to a new discipline, unified perceptual parsing, in Xiao et al (2018): The output of a DNN is not restricted to a main task but extended by a large set of related concepts, as demonstrated in their UPerNet architecture.

**Interpretable CNNs.** While the other approaches are supervised and rely on concept labels, Zhang et al (2018c) enforces in an unsupervised fashion the alignment of convolutional filters with concepts, which are in this case object parts. This is done by using filter-specific losses that encourage the filter to only activate locally around its maximum activation in the image. This assumes that each object part type occurs once in an input image.

### 4.1.2 Concept bottleneck models

General concept enforcement will ensure a set of interpretable outputs. So-called concept bottleneck models (CBM) additionally require that the output of a complete layer should be interpretable, i.e. all units should correspond to human interpretable concepts. CBMs primarily can be differentiated by the applied training scheme (important ones depicted in Figure 2).

**Concept whitening.** An example of a fine-tuning approach that re-trains a pretrained network is concept whitening (Chen et al, 2020). Concept whitening...
Table 2  Properties of concept analysis methods discussed in Subsubsection 4.1.2 according to the taxonomy defined in Subsection 3.2.

| Method                                      | Enforced Superv. | Model | Distance measure | Optim. | Label Type | Input |
|---------------------------------------------|------------------|-------|------------------|--------|------------|-------|
| Concept bottleneck models (Subsubsection 4.1.2) |                  |       |                  |        |            |       |
| Concept Whitening (Chen et al, 2020)        | ✓                | ✓    | linear           | dot    | LPQC       | any   |
| ProtoPNet (Chen et al, 2019a), CSPP (Feifel et al, 2021) | ✓                | -    | cluster          | $L_2$  | custom     | det   |
| Semantic bottlenecks (Losch et al, 2019)    | ✓                | ✓    | linear           | dot    | log. regr. | seg   |
| Concept bottlenecks (Koh et al, 2020)       | ✓                | ✓    | linear           | dot    | log. regr. | cls   |
| Weakly supervised CBMs (Belém et al, 2021)   | ✓                | ✓    | linear           | dot    | log. regr. | cls   |
| Concept Groups (Marcos et al, 2020)         | ✓                | ✓    | custom           | dot    | custom     | cls   |

suggests a replacement layer for batch normalization that is trained in a multi-task setting to apply batch whitening and align the dimensions of the latent space to given concepts. This is formulated as a linear programming problem with quadratic constraints (LPQC) and requires few epochs to disentangle the dimensions after replacing the batch normalization.

ProtoPNet. A clustering-based and unsupervised concept model approach is considered by Chen et al (2019a) in form of the ProtoPNet architecture. Here, the bottleneck layer consists of a prototype predictor: Windows in the CNN layer activation output are compared to unsupervised learned concept prototype CAVs, and the final output is derived from the resulting prototype scores. The CAV cluster centers and the rest of the model are trained jointly.

CSPP. An extension to object detection tasks was proposed with the Center Scale and Prototype Prediction (CSPP) architecture by Feifel et al (2021).

Semantic bottlenecks. The semantic bottlenecks architecture (Losch et al, 2019) also considers a fine-tuning training scheme. Here, the output of a complete layer of a pretrained DNN is linearly transformed to a representation where every filter represents one predefined concept, while the later layers are retrained.

CBM. Different schemes for directly training the concept bottleneck model with both the concept and the main objective were compared in Koh et al (2020). Settings were considered in which the part up-to the bottleneck and the part top-of the bottleneck were trained independently, jointly, or sequentially, as illustrated in Figure 2. Results revealed joint training as the tight
winner in performance. As in Losch et al (2019), performance was shown to be competitive to non-interpretable standard models without concept bottleneck, and also substantially more robust to spurious correlations with background features.

**Weakly supervised CBM.** Though Koh et al (2020) found that CBMs can mediocrely cope with small data tasks, especially the joint training requires a considerable amount of possibly costly concept labels. Therefore, Belém et al (2021) suggested a weak supervision of concept models by generating noisy labels from approximate rules when such are available from domain knowledge. In a fraud detection example setting, they found sequential training to work best, where first the noisy then the accurate labels are used.

**Concept Groups.** Another shortcoming of vanilla CBMs is that it may not be clear how a predefined concept from the bottleneck is used for the final output, respectively what its task-specific meaning is. To tackle this, Marcos et al (2020) suggests Concept Groups, a second bottleneck layer directly attached to the first one where nodes represent task-specific groups of concepts. These are obtained unsupervised, and the complete model is trained in a three-step sequential manner.

Lastly, it must be noted that the constraint imposed by a CBM, namely that single units in a layer correspond to interpretable concepts, does in general not guarantee that only information about those concepts is passed through the layer. Due to correlation of the concepts, further information can be encoded which is possibly non-semantic, as was shown and criticized in Mahinpei et al (2021).

### 4.2 Post-hoc concept models

Many applications require working with a pretrained DNN without changing its architecture. In such cases, post-hoc concept analysis methods are required that train concept models on given latent space outputs. The two main classes of methods to associate single concepts with latent space representations are supervised (concept localization) and unsupervised (concept mining) post-hoc
CA. Furthermore, we will discuss examples of the special case when a complete latent space is post-hoc disentangled on the basis of semantic concepts.

4.2.1 Concept localization

By now there is a formidable selection of supervised post-hoc concept analysis methods described in literature. For an overview, we cluster them by the model type into linear and non-linear models.

**Linear concept localization**

**NetDissect.** An early work on supervised post-hoc concept analysis, and basis for many further methods, was Network Dissection (NetDissect) by Bau et al (2017). They associate single filters of a convolutional DNN with one or several predefined concepts. To do this, upscaled and denoised activation maps of each filter were compared with ground truth concept segmentation masks, and the concepts with best agreement are picked. They also introduced the BRODEN dataset combination later often used as a baseline in other methods.

**Net2Vec.** A direct successor of NetDissect was Net2Vec (Fong and Vedaldi, 2018) where not a filter is associated to several concepts, but a concept is associated to a linear combination of filters. This is done by training a linear model to classify denoised activation map pixels into “belongs to concept” or “does not belong to concept”, resulting in binary segmentation masks. For the implementation (cf. Figure 4), a $1 \times 1$-convolution is used, the kernel weights of which are the CAV for the concept. For linear models like this the CAV points in the latent space direction of the concept as illustrated in Figure 3. Investigation of those CAVs for the first time revealed that such linearly obtained concept vectors behave like word vectors in word vector spaces, with cosine similarity encoding some semantic similarity.
## Table 3
Properties of concept analysis methods discussed in Subsubsection 4.2.1 according to the taxonomy defined in Subsection 3.2.

| Method                                      | Enforced Superv. | Model     | Distance measure | Optim. | Label type | Input |
|---------------------------------------------|------------------|-----------|------------------|--------|------------|-------|
| Post-hoc concept localization (Subsubsection 4.2.1) |                  |           |                  |        |            |       |
| NetDissect (Bau et al, 2017)                | - ✓              | linear    | dot              | picking| seg        | pixel |
| Net2Vec (Fong and Vedaldi, 2018), Schwalbe (2021) | - ✓              | linear    | dot              | log. regr.| seg        | pixel |
| Schwalbe and Schels (2020), Rabold et al (2020) | - ✓              | linear    | dot              | log. regr.| det        | window|
| TCAV (Kim et al, 2018), Chyung et al (2019) | - ✓              | linear    | dot              | SVM    | cls        | full  |
| CLM (Lucieri et al, 2020)                  | - ✓              | linear    | dot              | SVM    | seg        | full  |
| RCV (Graziani et al, 2018, 2020)           | - ✓              | linear    | dot              | LLS    | reg        | full  |
| CHAIN (Wang et al, 2020)                   | - ✓              | linear    | $L_2$            | Bregman| seg        | pixel |
| Local CAVs (Zhang et al, 2018b)            | - ✓              | loc. lin. | cosine           | Lasso  | seg        | window|
| AfI (Wu et al, 2020)                       | - ✓              | loc. lin. | dot              | custom | cls        | full  |
| SeVec (Gu and Tresp, 2019)                 | - ✓              | cluster   | cosine           | ?      | cls        | full  |
| CME (Kazhdan et al, 2020)                  | - semi cluster   | learned label spreading | mcls | full |
| IIN (Esser et al, 2020)                    | - (✓) DNN        | $L_2$     | custom           | any    | full       |
| CBM student (Haselhoff et al, 2021)        | - ✓              | linear    | cosine           | custom | cls        | full  |

**Net2Vec extensions.** There are several extensions of Net2Vec to concept center point prediction (Schwalbe and Schels, 2020; Rabold et al, 2020) instead of binary segmentation, and to object detection DNNs (Schwalbe, 2021). In both Schwalbe and Schels (2020) and Rabold et al (2020) a new ground truth encoding is used that highlights center points of object part concepts. This allows to learn center point prediction even if only binary segmentation masks are available, which is the case for most standard CA datasets. Schwalbe and Schels (2020) further suggests and compares different optimization settings for the concept model and suggests to increase the convolution kernel size from one pixel to a window, in order to provide more context for each single prediction. **Net2Vec for OD.** This is used and further evaluated in Schwalbe (2021), where efficiency is improved to apply a modified Net2Vec method to large object detector CNNs.
Figure 4 Exemplary linear concept localization model from Schwalbe (2021). The simple Net2Vec (Fong and Vedaldi, 2018) approach learns to predict segmentation masks for head using a $1 \times 1$-convolution followed by upscaling and normalization. The kernel vector $w_c$ then is the CAV. (Figure taken from (Schwalbe, 2021, Fig. 1))

TCAV. In parallel with Net2Vec, the similar method TCAV (Kim et al, 2018) for linear CAV retrieval was developed. Instead of single pixels they consider the complete activation map, and their linear support vector machine (SVM) concept model does image-level concept classification. They also suggest relative CAVs by training a concept model to differentiate just two concepts. Furthermore, in this work some concrete application of CAVs for fairness analysis are suggested and demonstrated which will be discussed later.

CLM. TCAV has also inspired several extensions. One of them is CLM by Lucieri et al (2020), where the concept classification is refined to a concept segmentation via the input attention to a concept output. The intriguingly simple approach achieved mediocre performance both for perturbation- and gradient-based heatmapping on a generated dataset and the CelebA dataset (Liu et al, 2015).

RCV. Another extension of TCAV concept models are Regression Concept Vectors (RCV) by Graziani et al (2018). Here, instead of binary classification, the linear model is trained to regress a continuous-valued concept using linear least squares (LLS) optimization. They also suggest an improved global concept-to-output attribution score (cf. Subsection 5.3) and demonstrate their approach on medical data in Graziani et al (2018) and Graziani et al (2020). The later work Graziani et al (2020) on RCVs, just as Kazhdan et al (2020), proposes to apply global average pooling to the full activation maps before training the linear classifier. This reduces the latent space and CAV size.

CHAIN. Not based on TCAV or Net2Vec, but also linear in nature, are the binary segmentation concept models proposed in the work on Concept-harmonized HierArchical INference (CHAIN) (Wang et al, 2020). Using Bregman iteration these are trained for a least squares distance to concept samples. The core idea of CHAIN is to assess the dependencies of CAVs in later layers with respect to CAVs in earlier layers. This turns a DNN into a concept graph of hierarchical inference.

Locally linear concept localization

Some CA methods do not rely on linear concept models, but still locally give rise to a linear interpretation and CAVs (loc. lin.).
Local CAVs. One such approach is pursued by Zhang et al (2018b) in order to locally represent outputs of a DNN by activation map vectors. They consider the derivative vector of the output with respect to the masked activation map. The mask for this purpose is learned globally for the respective output, using a Lasso-like optimization. Though the global concept model—containing the derivative function of the DNN—is highly non-linear, per-sample this still gives rise to comparable local CAVs.

AFL. Another approach, which is also locally producing CAVs, is Attacking for Interpretability (AFL) (Wu et al, 2020). Here, concepts represented in the final output classes of a classifier are located within activation maps. To obtain a CAV for an input instance and a selected output concept, they consider the local neuron-to-output attribution of neurons in a layer to the output of interest. The local CAV is the result of a global average pooling on the neuron attribution maps. In this case, the attribution is not defined via sensitivity, but as the difference between the vanilla and a perturbed version of the input, with perturbation done by a trained global attacker model.

Non-linear concept localization

SeVec. A simple clustering-based approach to obtain CAVs is followed by SeVec in Gu and Tresp (2019). Here, the (binarized) activation vectors for positive concept examples are clustered by cosine distance. The center of the most prominent cluster is taken as a CAV for the concept. From their diverse experiments, they report that there always was a dominant cluster containing most of the positive samples.

CME. Another example of CAVs from clustering under supervision was used for Concept-based Model Extraction (CME) by Kazhdan et al (2020). Their two specialties are that they also consider multi-class concepts like shape (with values, e.g., rectangle, triangle, circle), and that they assume that also unlabeled inputs are available for concept training. Thus, they use a semi-supervised multi-task learning approach, namely label spreading for spectral clustering\(^3\), to train their concept models. Similar performance results to Net2Vec are reported on the dSprites dataset (Matthey et al, 2017) and the Caltech-USCD birds dataset (Wah et al, 2011).

IIN. Other than the clustering-based approaches, Esser et al (2020) train a bijection between a layer’s output space to a vector space of the same size. The idea is that clusters of dimensions in that vector space represent given concepts. The bijection is realized by invertible DNNs, so-called normalizing flows, and termed Invertible Interpretation Network (IIN). An interesting label format is used: The image-level concept vectors are trained to be the difference vector between pairs of samples representing an increase of the concept (e.g., non-smiling → smiling). They also suggest to use their approach for concept mining by only enforcing independence of the dimension clusters.

\(^3\)See, e.g., the used implementation at https://scikit-learn.org/stable/modules/semi_supervised.html#label-propagation
Table 4 Properties of concept analysis methods discussed in Subsubsection 4.2.2 according to the taxonomy defined in Subsection 3.2.

| Method | Enforced Superv. | Model | Distance measure | Optim. | Label type | Input |
|--------|------------------|-------|-----------------|--------|------------|-------|
| Feature visualization (Olah et al, 2017; Nguyen et al, 2019) | - | linear | $L_2$ | - | seg | channel |
| ACE (Ghorbani et al, 2019), VRX (Ge et al, 2021) | - | cluster | $L_2$ | k-means | cls | full |
| Yeh et al (2020) | - | cluster | $L_2$ | custom | cls | full |
| NBDT (Wan et al, 2020) | ✓ | cluster | $L_2$ | HAC | cls | full |
| Explanatory Graph (Zhang et al, 2018a) | - | (cluster) | - | custom | det | window |
| NCAV (Zhang et al, 2021), Saini and Papalexakis (2020) | - | linear | $L_2$ | matrix fact. | seg | pixel |

CBM student. While all previous supervised methods assume full white-box access to the DNN of interest, Haselhoff et al (2021) break with this assumption and investigates how to obtain concept attribution from a black-box function. The idea pursued in the teacher-student approach in Haselhoff et al (2021) is to distill a concept bottleneck model from a trained function. Their student model is a concept bottleneck with a ResNet50 (He et al, 2016) back-end and a Gaussian discriminant analysis after the concept bottleneck. This allows a supervised concept analysis on black-box functions.

4.2.2 Concept mining

In literature, two method classes for finding concepts in latent space representations are prominent: Clustering-based approaches, and matrix factorization (matrix fact.) approaches. Examples of both are discussed in the following.

Concept mining using clustering

Feature Visualization. As for concept localization, the simplest approaches of unsupervised post-hoc concept analysis, or concept mining, are to investigate what concepts are encoded by single units of a DNN, like filters of a convolutional DNN. This is done in the broad spectrum of methods for feature visualization (Olah et al, 2017; Nguyen et al, 2019) where exemplary inputs or generated prototypes help to explain the meaning of such single units.

ACE. An approach respecting distributed representations of information is followed by Automatic Concept-based Explanations (ACE) in Ghorbani et al (2019) for visual concepts. They assume that meaningful visual concepts are represented by superpixels, i.e. connected patches, in images. Thus, they
cluster the latent space representation of size-normalized super-pixels using k-means clustering, and associate a concept with each cluster while the centers of the clusters serve as CAVs. (Yeh et al, 2020). The same approach is utilized by the direct successor by Yeh et al (2020), but with additional custom optimization criteria for the clustering. These shall ensure natural properties of concepts like spatial proximity of similar concepts. Also, they aim to capture a selection of concepts that covers the complete amount of information encoded in one latent space.

VRX. Another extension of ACE is the Visual Reasoning eXplanation framework (VRX) from Ge et al (2021). Before applying the super-pixel segmentation to an image, they mask out regions in an image that had little attribution to the output. For the attention scoring they use the standard heatmapping method Grad-CAM (Selvaraju et al, 2017).

NBDT. Other than previous k-means based methods, Neural-Backed Decision Trees (NBDT) (Wan et al, 2020) uses hierarchical agglomerative clustering (HAC) to find a hierarchy of CAVs in the last DNN hidden layer. The leaves of the hierarchical tree are concepts represented by the DNN outputs, with their CAVs being the respective weights from the last hidden layer. Using HAC with respect to $L_2$ distance on those leaves, a hierarchy of clusters is established. As before, the cluster center points are interpreted as CAV. For example, this hierarchy of CAVs can be used to define a decision tree surrogate model.

Explanatory Graph. A totally different approach that is loosely related to hierarchical and spectral clustering is pursued by the Explanatory Graph (Zhang et al, 2018a) extraction method. Their goal is to represent the inference of a CNN purely via a hierarchical graph of part objects and their part-relation: From small and simple concepts in earlier layers, to large and complex concepts in later layers. As constraints to define proper concepts, they assert that a concept prediction must (1) coincide with a high activation of a filter map; and (2) be spatially consistent with predictions of its parent concept in the successive layer. Due to this hierarchical dependency of concepts, they always produce a family of concept models that can only be inferred following the hierarchical structure. These concept models are each anchored and restricted to an image region.

Concept mining using matrix factorization

NCAV. A generalization of the previous clustering methods was proposed with Non-negative CAVs (NCAV) in Zhang et al (2021). They view k-means clustering as a special case of matrix factorization, and use this to find pixel-wise linear concept models for CNNs, i.e. linear weights for the convolutional filters. The idea of matrix factorization here is to find a global matrix $P$ (of size $\#\text{channels} \times \#\text{concepts}$) for a layer, where the columns of the matrix encode CAVs. For each input a matrix $S$ is obtained via optimization in a way that $S \cdot P$ approximately is the original activation map. $S$ then consists of the pixel-wise scores for the concepts, i.e. the per-pixel outputs of the concept models. The work compares three matrix factorization approaches, namely
k-means clustering, principal component analysis, and non-negative matrix factorization for ReLU nets, with most interpretable concepts found by the last one.

(Saini and Papalexakis, 2020). A similar approach to NCAV, also using non-negative matrix factorization, is pursued by Saini and Papalexakis (2020). The important difference is that they do not only associate concepts with filters (cf. dimensionality of $P$), but also input pixels and single neurons at once, leading to much more memory intensive optimization, but a little more direct association of concepts to input parts.

### 4.2.3 Complete latent space disentanglement

Some of the discussed methods allow not only to replace parts of the model but provide an (invertible) interpretable representation for a complete layer output. This is relevant if it is the aim to capture as much of the encoded information as possible, or to turn a model post-hoc into a concept bottleneck model. Some of the discussed methods are recapitulated here under this aspect.

Concretely, Yeh et al (2020) suggest a measure for evaluating completeness of a set of concepts: They intercept the connection between two layers by an interpretable intermediate output where each single dimension corresponds to one concept. While concept models are used to connect the earlier layer with the interpretable units, linear weights are learned to connect the interpretable representation with the next layer. They take the performance drop due to this interpretable interception as a measure for the completeness of the set of chosen concepts. Such an interpretable interception is also achieved by the matrix factorization approach of NCAV. Their idea to approximately represent the layer output as a product $S \cdot P$ of interpretable matrices allows to directly replace the layer output with this concept-based approximation. And the NBDT approach inherently ensures to capture all relevant information of the last hidden layer they consider: They take into account all weights connecting the last hidden with the output layer. Note that the supervised IIN method also achieves concept-based latent space disentanglement, but adding residual “non-semantic” dimensions as a fallback for encoded but not predefined concepts, to ensure invertibility.

### 5 Applications

This chapter provides an overview of core applications of concept analysis, and discusses interesting examples. The first sub-section 5.1 considers applications that utilize the additional concept outputs produced by concept analysis. The interactive model correction method of concept intervention is discussed in Subsection 5.2, and Subsection 5.3 gives an overview of useful metrics and approaches for qualitative verification based on CA.
Table 5 Overview of the presented model distillation approaches based on concept analysis outputs

| Distillation Method                        | Surrogate Model Type                         |
|-------------------------------------------|---------------------------------------------|
| CA & ILP (Rabold et al, 2020)             | Expressive rules                            |
| CME (Kazhdan et al, 2020)                 | Logistic regression, decision tree          |
| Additive explainer (Chen et al, 2019b)    | General additive model                      |
| Interpretable Basis Decomposition (Zhou et al, 2018) | Local linear model               |
| NBDT (Wan et al, 2020)                    | Decision tree (semantic hierarchies)        |
| Explanatory Graph (Zhang et al, 2018a)    | Hierarchical graph (only part-relations)    |
| CHAIN (Wang et al, 2020)                  | Hierarchical graph (inference dependencies) |
| VRX (Ge et al, 2021)                      | Graph DNN                                   |
| CBM student (Haselhoff et al, 2021)       | Concept bottleneck model                    |

5.1 Using enriched DNN output

Several applications require access to a rich set of features in the DNN (intermediate) output. Concept analysis provides methods to either enrich the output after training the model with few data samples, or directly and easily include rich semantic outputs into the architecture. We first discuss examples of model distillation utilizing concept analysis, and then verification methods that rely on these rich outputs.

5.1.1 Model distillation

By model distillation we understand the approximation of the functionality of the complete or parts of a DNN by a more interpretable model, which can be, e.g., a linear one or a decision tree (Arrieta et al, 2020). Model distillation into an interpretable surrogate model requires interpretable symbolic inputs for that surrogate model, such as color or age. However, many input domains for DNNs are non-symbolic, like images. Post-hoc attached concept model outputs can be used to provide the necessary symbolic input to the surrogate. This allows to replace bottom parts of the DNN similar to the fine-tuning approach used for the Semantic Bottleneck Models in Losch et al (2019) (cf. Figure 2). In the following, examples for different types of surrogate models are summarized. An overview is given in Table 5.

Rules and additive models

CA and ILP. For example, in Rabold et al (2020), the later layers are replaced by a set of rules learned using inductive logic programming. Also, the concepts are not located in one layer, but for each concept the layer with the best embedding is chosen.
CME. CME (Kazhdan et al, 2020) also considers all layers to find the best embedding of the predefined set of concepts. They, however, rely on simpler surrogate models, namely a linear one trained using logistic regression, and decision trees.

Additive explainer. Another example of an additive surrogate model for a classifier is the additive explainer model presented in Chen et al (2019b). As concept models they use the approach by NetDissect (Bau et al, 2017), in order to associate a predefined concept with the filter of a layer that mainly activates for this concepts. Chen et al (2019b) now trains a general additive model to predict the final classification output from those concept model outputs. For each instance, the general additive model predicts weights to linearly combine the concept model outputs.

Interpretable Basis Decomposition. A simple but local linear surrogate is considered in the Interpretable Basis Decomposition method (Zhou et al, 2018). They decompose a latent space vector representation of an input into a linear combination of CAVs. This is done by means of greedy least squares basis decomposition. Concretely, those local surrogates are then used to provide per-concept attribution heatmaps.

Hierarchical models

NBDT. The method NBDT (Wan et al, 2020) mines a hierarchy of CAVs, each of which represents the center point of a (sub-)cluster. They suggest to use this concept hierarchy to define a decision tree: Top-down, at each node one chooses the sub-cluster for which the representing CAV and the current activation vector have the smallest dot-product (note: not \(L_2\) distance as used for the clustering). To ensure good fidelity of the decision tree, a fine-tuning loss is tested that encourages the model to better sort activations into the correct clusters.

Explanatory Graph. Other than NBDT, which is restricted to the last layer, the Explanatory Graph method (Zhang et al, 2018a) discussed in Subsubsection 4.2.2 represents the complete model by a hierarchy of concepts. For this, they mine concepts from different layers. Here, the type of concepts and hierarchical relations are restricted to object parts and part relations.

CHAIN. Similarly, but without that restriction, the super-vised method CHAIN (Wang et al, 2020) produces a hierarchical inference graph. CHAIN linearly models how concepts in later layers depend on concepts in earlier layers. For this, pixel-wise linear CA models are used that provide CAVs. The main idea for obtaining the weights for linear dependency in CHAIN is to lift CAVs of later concepts to earlier layers. Weights are then trained to represent a lifted CAV as linear combination of CAVs from that layer.

Complex models

VRX. To capture and model both spatial and semantic relations between mined visual concepts, VRX (Ge et al, 2021) distills a graph neural network. As inference input, concepts are detected in the image (associated with image
patches), and a fully-connected graph of the matched patches is created that encodes spatial relationships and (learnable) semantic relationships of concept instances.

**CBM student.** An approach to distill an interpretable model from a classifier applicable without white-box access is chosen in Haselhoff et al (2021). As a surrogate, they train a concept bottleneck model with the part after the bottleneck being a decoder based on Gaussian discriminant analysis. This setup quite easily allows to determine the attribution of a concept to an output as the ratio of concept log likelihood and output class log likelihood.

### 5.1.2 Verification of symbolic properties

Besides model distillation, another usage of rich DNN output is for the verification of logical properties. Logical properties must be defined on symbolic features in the DNN (intermediate) output, which can be accessed using concept analysis. An exemplary verification of hierarchical relations like “dogs are mammals” is conducted in Roychowdhury et al (2018). They translate first-order logic rules into continuous-valued fuzzy logic rules that accept output scores of the DNN. The truth values of the rules can then be tested on a test set.

### 5.2 Concept intervention

For interactive human-machine-systems, like experts interacting with an assistant system, it may be helpful to allow an expert to correct intermediate steps in the model decision process. This can be done by changing the intermediate output of the model. However, to allow helpful intervention, an expert both needs to (1) understand the meaning of the intermediate output, as well as (2) be able to modify it according to symbolic knowledge. Part one is solved by using concept analysis methods. Part two can be tackled using so-called concept intervention. There are two approaches that rely on different prerequisites: (a) Either a vector representation of the concept must be available, or (b) the concept model output must directly influence later reasoning steps of the considered model.

**Concept model output intervention**

If the concept model output is part of the model inference process, the expert can manually change the output of the concept model and re-do the inference from the concept model output onwards. This is suggested and done for CBMs in Koh et al (2020). CME (Kazhdan et al, 2020) does this post-hoc for standard DNNs. They attach concept outputs post-hoc and then train a surrogate upon them. The surrogate decisions can now be intervened by changing concept outputs.
Concept representation intervention

The other setting for concept intervention is that a latent space vector is given that represents the direction towards a concept in the latent space. Then, the intermediate output vector in that latent space can be modified to point more or less into the direction of the concept. For example, projecting it to the plane orthogonal to the CAV eliminates the concept from the intermediate output. The modified vector can then be fed to the next layer. This approach is, e.g., used for the Counterfactual Explanation Score (CES) (Abid and Zou, 2021), where the difference between adding the concept and removing the concept is measured. In GAN dissection (Bau et al, 2018), the concept localization method NetDissect (Bau et al, 2017) is used to associate single units in a generative adversarial network for image generation with semantic concepts. Intervention—i.e. manipulation—of those unit values results in spatially local semantic manipulation of the created image.

5.3 Analysis of concept model properties

Concept analysis gives rise to some interesting qualitative and quantitative analysis options. These can be used to globally or locally verify a model by uncovering failure modes (Zhang et al, 2018b), or allowing for manual inspection of the rich semantics assessable via concept analysis. In the following, we first discuss concept-driven qualitative inspection methods enabled by CA (Subsubsection 5.3.1), and then quantitative measures related to CA results (Subsubsection 5.3.2).

5.3.1 Qualitative analysis methods

Some qualitative analysis methods are enabled by CA which are discussed in the following.

Local input-to-concept attribution. In the Interpretable Basis Decomposition approach (Zhou et al, 2018) the attribution of input pixels to a concept is visualized. For this, they use a standard and interchangeable heatmapping method (Grad CAM by Selvaraju et al (2017)), and treat the post-hoc attached concept model outputs as regular DNN outputs. They consider concepts that define a local basis for the output in order to semantically dissect the attribution to the final output. In CLM (Lucieri et al, 2020) also a perturbation based attribution method is applied and the heatmaps are used to allocate concept classification results to image regions.

Concept prototypes. For manual inspection, it may be interesting to get an impression of how a model “perceives” a localized or mined concept. For this, one can either provide examples (Ghorbani et al, 2019), patch examples to get a prototype (Ghorbani et al, 2019), or optimize a candidate to obtain a prototype for the concept. The latter is done in Kim et al (2018) by applying the DeepDream (Mordvintsev et al, 2015) optimization with respect to the concept outputs.
5.3.2 Quantitative properties

The following semantically grounded metrics directly arise from concept analysis.

Notation: We consider an exemplary DNN $f$ and a concept $c$ in layer $l$ with CAV $w_c$. $T$ denotes a test set of samples, and $p$ a single input sample. The DNN sub-function up to layer $l$ is denoted $f_{\rightarrow l}$, $f_{l\rightarrow}$ denotes the one from layer $l$ onwards, and—in case $f$ has multiple outputs—the function for the $k$th output of $f$ is written $f^k$.

**Concept embedding quality.** The following types of concept embedding quality measures are proposed in literature:

- As suggested in Schwalbe and Schels (2020), the best achievable performance of a concept model for a concept can be interpreted as the concept embedding strength or quality, i.e. how well information about the concept is embedded in the DNN. Standard performance metrics are, e.g., accuracy or $R^2$ for binary classification (Kim et al., 2018), and set intersection over union for binary segmentation (Fong and Vedaldi, 2018; Schwalbe, 2021).

- Misprediction overlap (MPO): In case of a family of concept models, Kazhdan et al. (2020) argues that it is important to assess the distribution of errors over concepts. They suggest to measure the misprediction overlap as the proportion of test samples for which at least $n$ relevant concepts are mispredicted.

**Concept similarity.** As discussed in Subsection 3.2, there are several approaches to measure the similarity of concept embeddings in the case CAVs are available. These usually rely on CAVs residing in the same layer, even though CAV-lifting can be performed to also compare concepts embedded in different layers as done in Wang et al. (2020). The embedding similarity can be compared with prior knowledge on the ground truth semantic similarity for verification purposes as done in Schwalbe (2021). Here, one has to differentiate between globally and locally available CAVs:

- As discussed in Subsection 3.2, global CAVs are often compared using one of cosine similarity (e.g., Fong and Vedaldi (2018); Schwalbe (2021); Kim et al. (2018)) or $L_2$ distance (e.g., Ghorbani et al. (2019); Yeh et al. (2020); Wang et al. (2020)).

- For the local CAVs used in Zhang et al. (2018b), the authors suggest to assess the distribution of concept relation values given a test set $T$. As measure of concept similarity for CAVs in the same layer they consider cosine distance. They assume a prior distribution of values and apply Kullback-Leibler divergence to compare this with the measured distribution.

**Local concept-to-output attribution.** Given a sample, there are several suggestions on how to quantify the attribution of a concept embedding to an output (or another concept model output).

- **Local TCAV score:** Kim et al. (2018) measures local sensitivity (Baehrens et al., 2010) of an output with respect to a CAV by measuring the partial
derivative along the CAV:

$$\text{TCAV}(f; c \rightarrow k)(p) := \nabla f^k_{l \rightarrow i}(f \rightarrow l(p)) \cdot w_c$$  \hspace{1cm} (1)

- **Counterfactual explanation score (CES):** To robustify the TCAV sensitivity score, Abid and Zou (2021) suggests to use an approximation of the direct derivative via a step-perturbation. Using concept intervention (cf. Subsection 5.2), they add the concept of interest by moving the latent space vector one step into the direction of the CAV. For a step size $\delta$ (originally 10,000) the approximation is then

$$\text{CES}(f; c \rightarrow k)(p) := f^k_{l \rightarrow i}(f \rightarrow l(p) + \delta w_c) - f^k(p).$$

- The CHAIN method by Wang et al (2020) assesses the local hierarchical dependency of pixel-wise CAVs in later layers to CAVs in earlier layers. They suggest to use the partial derivative of a concept output along the CAV of an earlier-layer concept as local concept-to-concept attribution.

- An approach not relying on CAVs is to find a linear surrogate model based on concept outputs that directly provides concept-to-output attribution weights, as is done in a local fashion in Chen et al (2019b).

**Global concept-to-output attribution.** Local concept-to-output attribution values can be aggregated on a test set $T$ to an approximate global attribution value. While this was first suggested in Kim et al (2018), the aggregation method was refined in later work:

- The original way to aggregate local TCAV scores as defined in Equation 1 to a global TCAV score was proposed in Kim et al (2018). The metric is specific to classifiers since it relies on a partition of the test set $T$ into sub-

  $$\text{TCAV}_{\text{global}}(f; c \rightarrow k) := \frac{1}{\#T_k} \sum_{p \in T_k} \mathbb{1}_{\text{TCAV}(f; c \rightarrow k)(p) > 0}$$  \hspace{1cm} (2)

- The normalized bidirectional relevance (NBR) is an improved version of Equation 2 suggested in Graziani et al (2018). They aggregate local sensitivities as: (1) the mean sensitivity $\mu_{c \rightarrow k} = \text{mean}_{p \in T_k} \text{TCAV}(f; c \rightarrow k)(p)$ for an output class $k$ over samples $T_k$ of that class, (2) weighted by the concept model’s R-squared value $R^2_c$, and finally (3) normalized by the standard deviation $\sigma_{c \rightarrow k}$ of the sensitivity:

  $$\text{NBR}(f; c) := \frac{R^2_c \cdot \mu_{c \rightarrow k}}{\sigma_{c \rightarrow k}}$$  \hspace{1cm} (3)

This yields stronger sensitivity for accurate concept models and such with less output variance (Graziani et al, 2020).
• The CHAIN method lifts CAVs from later layers to an earlier layer in order to represent the lifted CAV as linear combination of CAVs in this earlier layer. These global concept hierarchical inference weights are further used to define a surrogate model (cf. Subsubsection 5.1.1).
• Sometimes, one is interested in the influence of concept $c_A$ on concept $c_B$, however, has no concept model for $c_A$, but only concept samples. In this case, both the AfI framework (Wu et al, 2020) and Schwalbe (2021) suggest to observe the discrepancy in $c_B$’s output between a set of samples with $c_A$, and a set without $c_A$. In Schwalbe (2021) the discrepancy is simply measured as the discrepancy in performance of $c_B$. AfI measures the maximum mean discrepancy (MMD) (Gretton et al, 2012), a standard measure to compare two distributions, between the output distributions of $c_B$ on the different input datasets.

Local concept interactions. One might be interested in the local interaction of concepts $c_A$ and $c_B$, i.e. how the local attribution of $c_A$ to an output will change with changes to $c_B$. In case of CBMs, or if $c_A$ and $c_B$ have a CAV in the same layer, standard interaction analysis methods can be applied, such as integrated Hessians (Janizek et al, 2020).

Concept embedding validity. As was already found in Kim et al (2018) and confirmed in Rabold et al (2020), especially linear (supervised) concept models are non-robust with respect to outliers, and the training may not be stable. Thus, measures are necessary that confirm whether a found CAV is a stable and meaningful solution or not:
• In Kim et al (2018) a t-test is used to check whether several CAVs trained for the same concept behave consistently.
• In Pfau et al (2021) a hypothesis test is used that checks whether the concept sensitivity is higher than that of a reference noise vector. This is also applicable to check validity of mined CAVs.

In Rabold et al (2020) an ensembling approach is suggested to stabilize linear models. An invalid or instable concept embedding may unmask an inconsistently defined concept, or an inappropriate CA method.

Concept intervention scores. The concept intervention used in Koh et al (2020) (manually changing the bottleneck outputs of CBMs) may serve to measure the influence of wrongly predicted concepts onto the final decision. In that work they compare the performance of the original CBM with CBMs with an increasing rate of concepts being intervened, i.e. their concept bottleneck outputs being replaced with ground truth labels. They found that for most concepts the correct prediction is substantial for correct output of the final model (cf. (Koh et al, 2020, Fig. 4)). Concept intervention scores can also be seen as a local concept-to-output attribution measure that is perturbation-based and specific to CBMs.

Concept completeness. The notion of concept completeness was introduced in Yeh et al (2020). It measures how much of the task-relevant information encoded in a DNN is covered by a set of concept embeddings.
They suggest to measure this as the decrease in model performance when turning it post-hoc into a concept bottleneck. The bottleneck is inserted between layers $l$ and $l+1$ as follows: First, the bottleneck layer after $l$ is inserted, with the connections from $l$ to the bottleneck concept outputs being the concept models. Then, weights are learned to connect the bottleneck to the next layer $l + 1$. This differs from Semantic Bottlenecks (Losch et al, 2019), where the complete part $f_{l\rightarrow}$ is replaced and retrained. While the original method from Yeh et al (2020) assumes the existence of linear models defined by CAVs, the performance discrepancy can be measured for any other method that post-hoc inserts a bottleneck (cf. Subsubsection 4.2.3).

**Concept interpretability.** Due to the distributed representations occurring in a DNN, one unit, respectively one filter in case of CNNs, may be involved in representing several semantic concepts. In the work on NetDissect, Bau et al (2017) suggest to take the amount of these concepts as a measure for the interpretability of the filter. Fong and Vedaldi (2018) inverted this and took sparsity of a CAV (i.e. how many filters are needed to encode the concept) as a measure for the interpretability, or disentanglement, of the concept representation (cf. Subsection 3.2).

### 6 Image datasets for supervised CA

In this chapter we collect and compare different datasets that so far have been used for supervised concept analysis methods presented in Section 4. This is meant as a reference for researchers in search of suitable datasets for evaluating CA approaches, and to demonstrate the breadth of application fields. A tabular overview of the datasets and their key properties is compiled in Table 6.

Datasets are classified as follows: We start in Subsection 6.1 with datasets of diverse real world images that are suitable for practical baseline evaluation of DNNs for complex computer vision tasks. Next, in Subsection 6.2, a collection of domain specific image concept datasets are presented, that can serve for evaluation of domain specific applications, or of CA methods on more complex tasks. Lastly, an overview of “toy” and simple image datasets is given in Subsection 6.3 that contain few simple concept classes like shapes, textures, or colors. These may serve for initial experimentation or comparison.

#### 6.1 Large and diverse real-world image datasets

The following large real-world image datasets with concept annotations are used throughout several papers to establish a performance baseline for CA approaches (Fong and Vedaldi, 2018; Kim et al, 2018; Schwalbe, 2021). They are suitable for practical evaluation of large DNNs in complex computer vision applications like object detection (Schwalbe, 2021).

**ImageNet.** ImageNet (Deng et al, 2009) is a popular and large image dataset that aims to provide sample images for the abundance of 80,000 hierarchical lexical synonym sets defined in the WordNet lexical database (Fellbaum, 1998). ImageNet features more than 3.2 million samples with binary classification
Table 6: Overview of image datasets used for supervised concept (C) analysis. Besides concept type and label type, we collected the number of samples, concept classes, and the number of samples per least dominant class value of the concept. Abbreviations: attr.=attributes, avg.=average, equ. dist.=equally distributed.

| Name                          | C Label Type     | C Types                              | # Samples | # C Classes | # Samples / C Class |
|-------------------------------|------------------|--------------------------------------|-----------|-------------|--------------------|
| Large diverse datasets (Subsection 6.1) |                  |                                      |           |             |                    |
| ImageNet (Deng et al, 2009)   | cls,det          | objects, parts                       | 3 000 000< | 5247        | 600 avg.           |
| BRODEN (Bau et al, 2017)      | seg,cls          | all                                  | 63 305    | 1197        | 10 ≤               |
| BRODEN+ (Xiao et al, 2018)    | seg,cls          | all                                  | 57 095    | 1002        | 20 ≤               |
| MS COCO (Lin et al, 2014)     | seg              | body parts                           | 118 287   | 9           | 40 000 ≤           |
| Domain specific datasets (Subsection 6.2) |                  |                                      |           |             |                    |
| LFW (Huang et al, 2008)       | cls              | gender                               | 13 233    | 1           | -                  |
| LFWA+ (Liu et al, 2015)       | cls              | facial attr.                         | 13 233    | 40          | -                  |
| CelebA (Liu et al, 2015)      | cls              | facial attr.                         | 202 599   | 40          | -                  |
| FASSEG (Khan et al, 2015)     | seg              | facial parts                         | 270       | 3           | -                  |
| Picasso (Rabold et al, 2020)  | seg              | facial parts                         | 452       | 3           | 452                |
| Knee X-Rays (Koh et al, 2020) | cls              | clinical attr.                       | 36 369    | 10          | 5% ≤               |
| CUB (Wah et al, 2011)         | cls,det          | bird attr./parts                     | 11 788    | 327         | 100%               |
| Simple datasets (Subsection 6.3) |                  |                                      |           |             |                    |
| GTSRB (Stallkamp et al, 2011; Schwalbe and Schels, 2020) | seg | color, shape, part                  | 50 000<   | 10          | 211 ≤              |
| A-GTSRB (Stallkamp et al, 2011; Kronenberger and Haselhoff, 2019) | cls | color, shape, part                  | 70 000<   | 32          | 211 ≤              |
| FMD (Sharan et al, 2014)      | cls              | material                             | 1000      | 10          | 100                |
| Google-512 (Schauerte, 2010)  | cls              | color                                | 5632      | 11          | 512                |
| dSprites (Matthey et al, 2017) | cls,det          | shape, spatial                       | 737 280   | 4           | equi. dist.        |
| 3dshapes (DeepMind, 2021)     | cls              | shape, spatial                       | 480 000   | 6           | equi. dist.        |
| SCDB (Lucieri et al, 2020)    | seg              | shape                                | 6000      | 10          | equi. dist.        |
labels for 5247 hierarchically related synonym sets. The number of samples per synonym set varies a lot, with an average of 600 samples per set, and 50% of the sets containing more than 500 samples. Selected concept classes served, e.g., for validation purposes in the TCAV paper by Kim et al (2018).

Source: https://image-net.org/

BRODEN. The BRoadly and DEnsely labeled dataset (BRODEN) was first introduced in Bau et al (2017). It unifies diverse other image datasets (ADE20k by Zhou et al (2017), OpenSurfaces by Bell et al (2014), Pascal-Context by Mottaghi et al (2014), Pascal-Part by Chen et al (2014), and the Describable Textures Dataset by Cimpoi et al (2014)). In total, Broden features 63,305 different images resized to unified resolution $224 \times 224$, $227 \times 227$, or $384 \times 384$. With 1197 classes in total, the dataset labels encompass pixel-wise concept segmentations of types color (11), texture (47), material (32), object (584), part object (234), and classification labels for 468 scene type concepts. The amount of labels varies greatly, going down to as few as 10 samples per class.

Source: https://github.com/CSAILVision/NetDissect

BRODEN+. In Xiao et al (2018) the original BRODEN dataset was re-worked to make classes more distinct, and feature a sufficient number of samples per class to serve for DNN training. Mainly, they merged highly similar concept classes, removed color classes and classes with too few samples, and renamed labels to match the naming in the Places dataset (Zhou et al, 2014). This results in 57,095 image samples and 1002 classes in total.

Source: https://github.com/CSAILVision/unifiedparsing

MS COCO Bodyparts. The Microsoft Common Objects in COntext object detection dataset (MS COCO) (Lin et al, 2014) features over 1.7 million keypoint labels for over 150,000 person instances in 118,287 training and 5000 validation images with comparatively high resolution. Schwalbe (2021) suggests and demonstrates a general method to turn person keypoint labels into CA-ready segmentations of body parts described by keypoints (here: eye, nose, ear, arm, leg, wrist, ankle, shoulder, hip).

Source: https://cocodataset.org/

6.2 Domain specific image datasets

This section collects several domain specific real-world image datasets that have so far been used for use-case specific evaluation of CA methods. Since the collection is dominated by concept datasets for facial features annotated in portraits, these are gathered into their own subsection (Subsubsection 6.2.1) and discussed first. Then, two further examples of detailed labeled domain specific datasets are presented in Subsubsection 6.2.2.

6.2.1 Facial features concept datasets

The following facial features datasets have served for CA evaluations:

LFW. The Labeled Faces in the Wild (LFW) dataset (Huang et al, 2008) features 13,233 portraits of 5749 people with labels of name and gender. It was
used by Kim et al (2018) in the fairness evaluations of the TCAV method. 

Source: http://vis-www.cs.umass.edu/lfw/

**LFWA+**. The LFWA+ dataset provides the CelebA additional label types of 5 landmark locations and 40 binary attributes for the original LFW image samples. It was introduced in Liu et al (2015) alongside the CelebA dataset. 

Source: https://mmlab.ie.cuhk.edu.hk/projects/CelebA.html

**CelebA**. The Large-scale CelebFaces Attributes (CelebA) dataset (Liu et al, 2015) contains 202,599 portraits of 10,177 celebrities annotated with 5 landmark locations and 40 different binary attributes, like bald, mustache, and makeup. It was used, e.g., in Lucieri et al (2020) for evaluation of the concept localization method CLM on a model trained on CelebA for gender classification. The same label classes are used as in the LFWA+ dataset. 

Source: https://mmlab.ie.cuhk.edu.hk/projects/CelebA.html

**FASSEG**. The FAce Semantic SEGmentation dataset (Khan et al, 2015) contains 70 frontal face and 200 multi-pose face images with semantic segmentation of the object part concepts eye, nose, mouth. The portraits are sections from images taken from the MIT-CBCL (for Biological and Computational Learning, CBCL), FEI (Thomaz and Giraldi, 2010), and Pointing04 (Gourier et al, 2004) datasets. FASSEG served as a basis for the generated dataset used in Rabold et al (2020) for CA-based surrogate model creation. 

Source: http://massimomauro.github.io/FASSEG-repository/

**Picasso**. In Rabold et al (2020) the generated Picasso dataset is presented for binary classification of images into “valid” and “invalid” face. In each image, clips of facial features (eye, nose, mouth) from the FASSEG dataset (Khan et al, 2015) are pasted upon portrait images in which facial features were erased. The arrangement of the features is considered an “invalid” (scrambled) face if the feature arrangement is unnatural, e.g., eye and nose swapped. For concept segmentation labels, the original segmentation information was retained. For each concept, 452 training samples and 48 test generated samples were used. 

Source: https://github.com/mc-lovin-mlem/concept-embeddings-and-ilp/tree/ki2020

### 6.2.2 Other domain specific image datasets

In the following, two other examples of domain specific image datasets are described that feature interesting concept labels. 

**Knee X-Rays**. For CBM training, in Koh et al (2020) a clinical dataset of diagnosis from knee X-ray images was used. The dataset was compiled by the Osteoarthritis Initiative (Initiative, 2021). The dataset prepared by Koh et al (2020) consisted of 36,369 X-ray observations of 4,172 patients, at a high uniform resolution of 512 x 512 pixels. Koh et al (2020) filtered highly unbalanced concepts. Only those were included where more than 5% of the images feature the non-dominant class. In addition to the multi-value diagnosis classification, binary labels for further 18 other clinical concepts are included. 

Source: https://nda.nih.gov/oai
CUB. The Caltech-UCSD Birds-200-2011 (CUB) dataset (Wah et al, 2011) consists of 11,788 bird images with classification annotations for the 200 contained bird species, and additional annotations of 15 part locations, 312 binary attributes (e.g., wing color, beak shape) with visibility information, and the bounding box of the depicted bird. The dataset was used, e.g., for CBM training in Koh et al (2020), and for concept localization in CME (Kazhdan et al, 2020).

Source: http://www.vision.caltech.edu/visipedia/CUB-200-2011.html

In TCAV, the medical use-case of predicting diabetic retinopathy from retinal fundus images was analyzed with respect to diagnostic concepts like microaneurysms or pan-retinal laser scars. However, the concept data is not freely available.

6.3 Simple evaluation datasets

While large real-world datasets may be interesting for a practical evaluation of DNNs or CA methods, simpler settings are preferred for initial method evaluation and comparison. Thus, the following subsection collects several small-resolution datasets that concentrate on annotations for simple concepts like shape, color, and texture. The examples are classified into datasets based on real-world images (Subsubsection 6.3.1) and artificial ones using generated samples (Subsubsection 6.3.2).

6.3.1 Simple real-world concept datasets

The following examples of real-world datasets provide annotations for simple concepts and can be used to validate small computer vision DNNs using CA.

GTSRB. The German Traffic Signs Recognition Benchmark (GTSRB) dataset (Stallkamp et al, 2011) is a classification dataset that features 43 classes of traffic signs, distributed onto more than 50,000 small (15 × 15 pixels) to middle (250 × 250) sized real world images. All images are close-up and fairly frontal, and the labels provide the exact bounding box of the contained sign. The bounding box labels allow to transform images to centered and uniformly sized sign photo sections. This was utilized in Schwalbe and Schels (2020) to automatically annotate bounding boxes for contained letters, by using static positions. This served as simplistic setting for evaluating different CA methods.

Source: https://benchmark.ini.rub.de/gtsrb_dataset.html

A-GTSRB. For the experiments in Kronenberger and Haselhoff (2019), an augmented version of the GTSRB dataset was created, enlarging it by about 60% and adding classification labels for diverse concept types: main color and border color (5 values each), shape (4), and contained letters (10) and symbols (13). The new data samples were created by domain randomization (new combinations of shape and color) and background randomization (adding patches to the background).

Source: https://benchmark.ini.rub.de/gtsrb_dataset.html
FMD. The Flickr Material Database (FMD) (Sharan et al, 2014) provides each 100 images for ten common material classes. It was used alongside the Describable Textures Dataset (Cimpoi et al, 2014) contained in BRODEN (Bau et al, 2017), and the Google-512 dataset (Schauerte, 2010) for evaluation in the SeVec concept localization method paper Gu and Tresp (2019).

Source: https://people.csail.mit.edu/lavanya/fmd.html

Google-512. The Google-512 dataset (Schauerte, 2010) consists of 512 sample object images for each of 11 basic color terms, collected using the Google search engine. It was used in Gu and Tresp (2019) for color concept localization.

Source: https://cvhci.anthropomatik.kit.edu/~bschauer/datasets/google-512/

6.3.2 Simple artificial concept datasets

Finally, we collect some simple artificial image datasets that allow for first evaluations and comparisons of concept models.

dSprites. The dSprites dataset (Matthey et al, 2017) is a popular simple artificial dataset for evaluation of latent space disentanglement methods. It consists of images in which a geometric shape is pasted onto a black canvas, with the following varying (discretized) latent factors: shape (3), scale (6), orientation (40), and position (each 32 values for $x$- and $y$-position). The dataset contains images of all 737 280 possible combinations of the latent factors, in low resolution of $64 \times 64$ pixels. In Kazhdan et al (2020) the dataset was considered for evaluation of concept localization and CBM methods.

Source: https://github.com/deepmind/dsprites-dataset/

3dshapes. Similar to dSprites, 3dshapes (DeepMind, 2021) is an artificial dataset generated via varying a fixed set of latent factors, originally used and intended for unsupervised disentanglement research (Kim and Mnih, 2018). The 480 000 samples of size $64 \times 64$ pixels each depict a 3D geometric shape centered within a rectangular room, with varying floor, wall, and object color (each 10 hue values), as well as object scale (8), shape (4), and camera orientation (15 values). The dataset was used in Kazhdan et al (2021) for comparison of CA methods with disentanglement methods.

Source: https://github.com/deepmind/3d-shapes

SCDB. The synthetic Simple Concept DataBase (SCDB) for binary image classification was presented in Lucieri et al (2020) in order to mimic challenges in skin lesion classification using dermatoscopic images. It contains 6000 samples for concept training with circular binary segmentation masks of 10 shape concepts. Each image contains one large geometric shape placed on black background, which contains and is surrounded by smaller geometric shapes which represent the labeled concepts. Class labels of the two classes are determined by simple disjunctive predicate rules on co-appearance of small shapes, e.g., ($\text{hexagon} \land \text{star}) \lor (\text{ellipse} \land \text{star}) \lor (\text{triangle} \land \text{ellipse} \land \text{star})$. The position, rotation, color, count, as well as appearance of two task unrelated small shapes
are randomized.

Source: https://github.com/adriano-lucieri/SCDB

7 Challenges and research directions

The previous chapters provided a broad overview of investigated methods, applications, and datasets. On this basis, this section gives some possible further research directions to enrich the field of concept analysis, and foster its practical application.

Method combinations

As can be seen from Tables 1–4, not all combinations of properties for concept localization are fully leveraged so far. Further non-linear models like clustering may be promising for supervised concept analysis, and unsupervised concept analysis methods are still scarce, despite their value for qualitative explanations. Also, further investigation of mining segmentation or detection concept models may be valuable. And finally, further investigation in detection approaches may be promising to enable less texture-focused localization: Other than segmentation, they use more concept information (more than one activation map pixel).

Linear models and clustering

Concept localization using linear models suffers from inherent instability: The hyperplane defining the concept model strongly depends on the support points. A solution may be ensembling of models (Rabold et al, 2020). Furthermore, Goyal et al (2019) showed that linear models like TCAV (Kim et al, 2018) are mostly overconfident and may require additional confidence calibration. For concept mining approaches, a big challenge is to find suitable concept candidates. The mined concepts should both be relevant to the model functioning, and meaningful to humans. The current superpixeling approaches used for clustering approaches may not capture all types of concepts, and in general need not to be well align with human intuition on a concept. Moreover, other methods like matrix factorization cannot guarantee meaningfulness of the obtained concepts (Zhang et al, 2021). Hence, for concept mining, further priors and constraints could help to improve meaningfulness for humans. To give an example, one could use tracking information from temporal sequences to find independently moving sub-parts of objects.

Completeness and minimality

When using concepts to explain the inner workings of a model as in Rabold et al (2020), it is desirable to have a set of concepts that is both minimal and complete. It is unclear how to achieve completeness in supervised setting (what concepts are still missing?). And minimality is likewise hard to achieve because solutions for picking a generating set of concepts are not unique with both concepts and their CAVs not being independent.
Other domains and architectures

Finally, it would be an interesting challenge to apply concept analysis to other domains and to other DNN architectures than standard single-frame visual tasks. Examples may be video processing, audio or text processing with transformers. Concepts for text and audio might be emotions, single words or typical sentence constructions. Also, the networks analyzed are usually small and far from sizes needed for some important applications like automated driving perception. Only two of the presented methods consider complex tasks like object detection: CSPP (Feifel et al., 2021) and Schwalbe (2021), the latter uncovering severe performance issues for extension to larger models in the baseline method Net2Vec (Fong and Vedaldi, 2018).

Assessment applications

As shown in Schwalbe (2021), concept analysis is suitable for diverse verification methods applicable in domains where responsible AI, and thus thorough functional assessment, is relevant. It promises to both provide semantic alignment of DNN intermediate outputs and quantitative measures that allow to define local and global performance indicators, easing automatic assessments. More practical evaluations could be a great guideline to improve upon the suggested metrics, find meaningful reference values, and finally fill gaps in current DNN assessment recommendations.

Availability of data

A challenge common to all types of supervised concept analysis: Richly and densely annotated data is required like in the combined Broden dataset from Bau et al. (2017), which means high labeling effort.

8 Conclusion

After a rapid development over the last years, concept embedding analysis has matured to an interesting sub-field of explainable artificial intelligence. This survey has established a common definition of efforts and related terms. Specifically, CA is roughly summarized as associating semantic, human interpretable concepts to intermediate output representations of deep neural networks (DNN), by means of simple helper concept models. To allow comparison of related approaches, a taxonomy is suggested that, amongst others, differentiates the types, inputs, outputs, and supervision of concept models.

Using this scheme, more than 30 divers CA methods are reviewed, categorized, and compared, providing a broad overview of approaches for CA. This should provide a good starting point for researchers seeking to position their CA related methods, or looking for ones that suit their use-case. Applications and use-cases are also gathered and discussed in detail. The most often encountered one is model distillation using concept outputs. Nevertheless, other interesting applications are found and reviewed, like intervention of concept outputs for interactive human-machine-systems, and verification relying either
on the additional concept outputs, qualitative assessments, or metrics arising from CA results. An extensive list of metrics occurring in literature is compiled that allows to easily find appropriate measures for DNN assessment using CA. For the practical entrance to the topic, a broad collection of image datasets with concept labels useful for evaluation of CA methods is provided. Datasets are classified according to their use-cases in CA research. Relevant statistics and traits are summarized, showing that many helpful resources are currently available.

Altogether, this review should give researchers interested in applications or methods for semantic DNN latent space assessment a good starting point, and clearly establish the XAI sub-field of concept embedding analysis. We look forward to more interesting results in the field, especially with respect to the identified open research challenges: more datasets; improvement of the linear and unsupervised clustering approaches; selecting a good set of concepts for explaining a DNN (especially one that is both minimal and complete); and leveraging CA in further practical and complex use-cases and applications.

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