

Testing with Concept Activation Vectors (TCAV)

Ivan Rodriguez

October 26, 2023

Kim et. al., “Interpretability beyond feature attribution: Quantitative Testing with Concept Activation Vectors (TCAV)”. In ICML - PMLR (2018). [github](#)

What is TCAV ?

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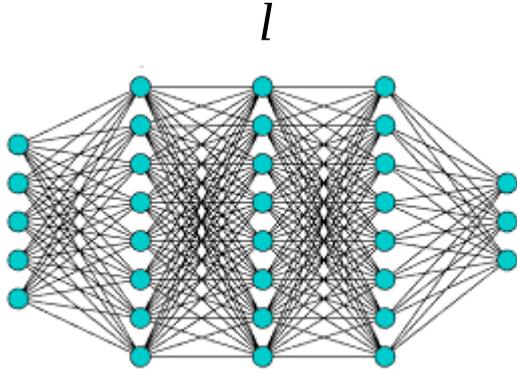
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- TCAV describes the relationship between a concept and a class rather than explaining a single prediction, providing valuable global interpretation of a model’s behavior.
- TCAV is primarily applied to DNNs, but it has the potential to work with any model where calculating directional derivatives is feasible (more clarity on this later).

TCAV idea

Given a trained DNN (regressor or classifier):

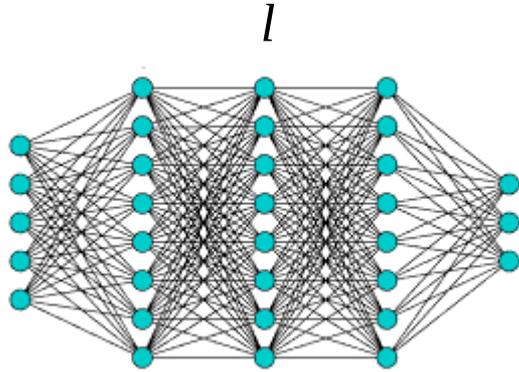


Devise a method to measure how sensitive is a given layer, l , to a certain concept that could describe our data.

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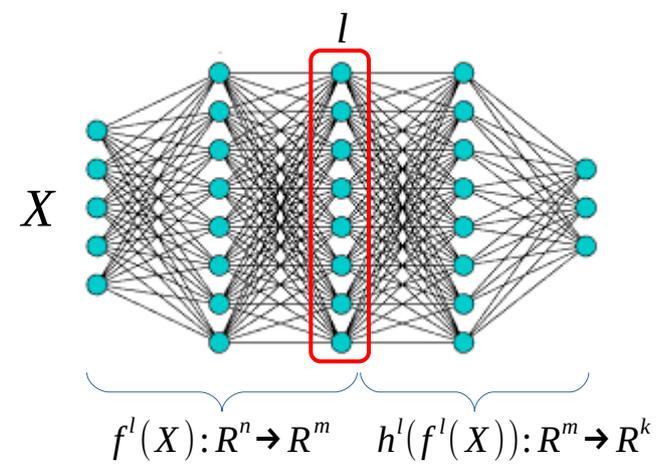
The paper proposes a simple and interesting approach through what they call:

Concept Activation Vector (CAV)

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Recipe to create a CAV

1 – select layer l with output $f^l(X) \in R^m$

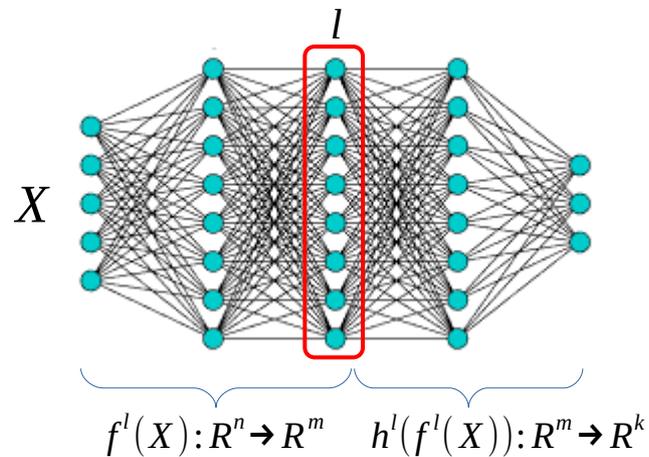


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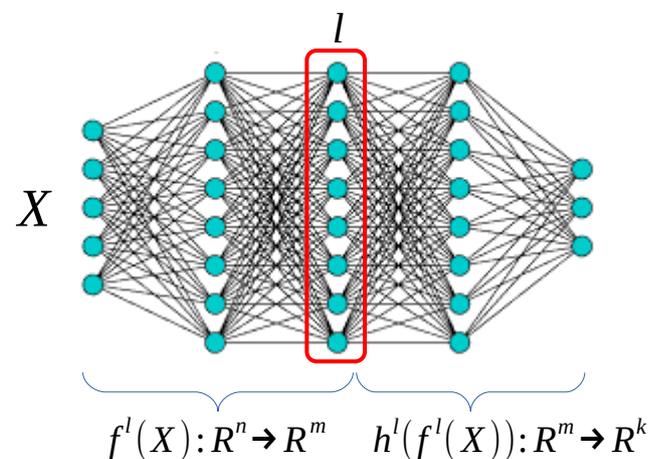
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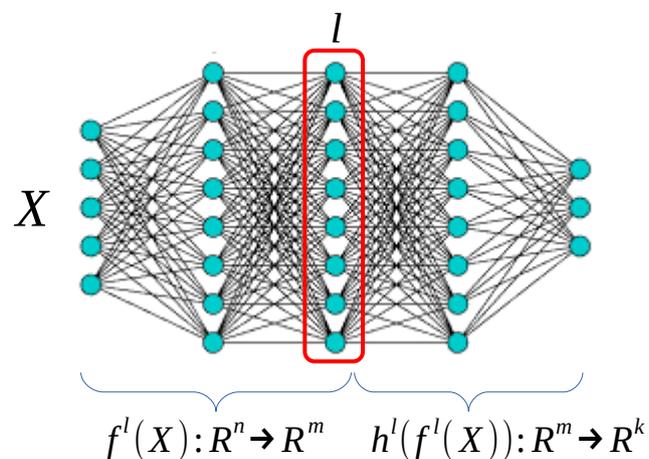
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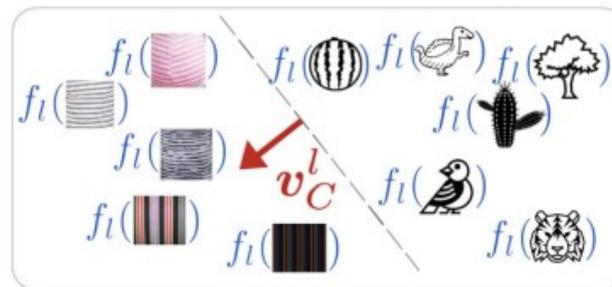
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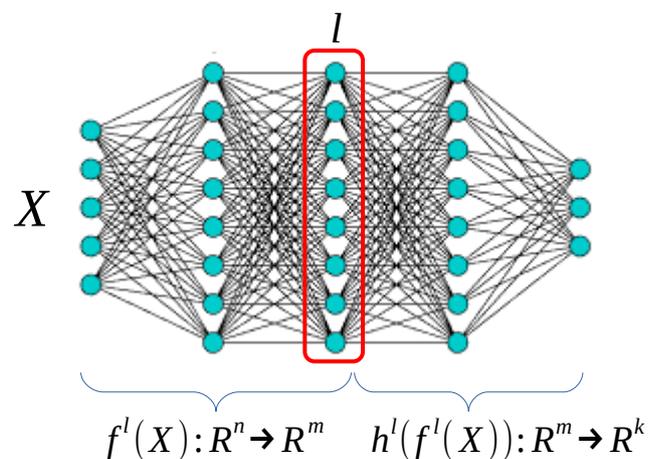
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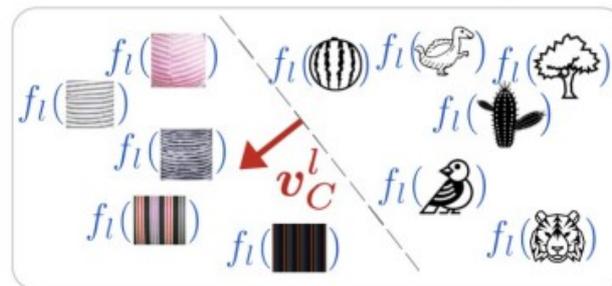
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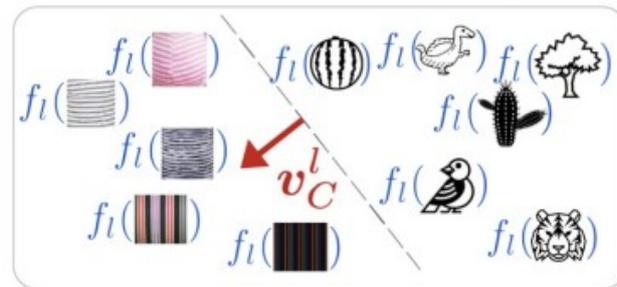
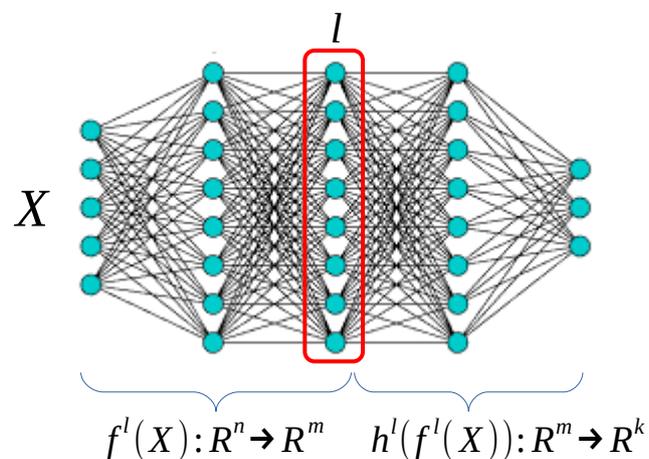


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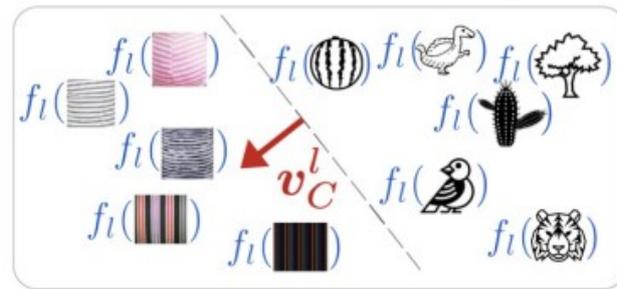
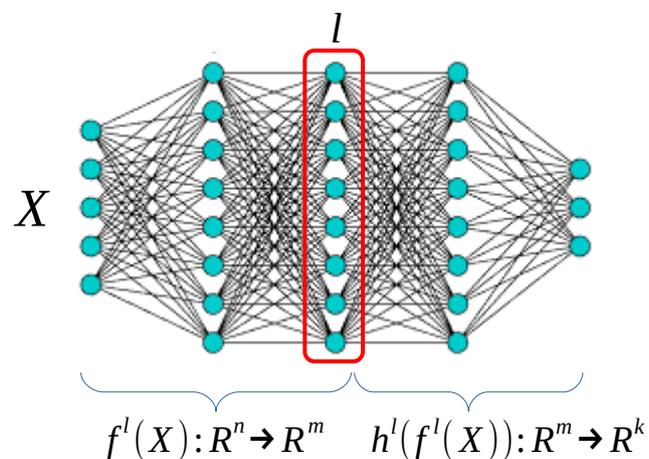


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$S_{C,k,l}$: In other words how important is the concept C in layer l for predicting the class k

TCAV Score

Let k be a class label for a given supervised learning task and let X_k denote all inputs with that given label. We define the TCAV score to be:

$$TCAV_{Q_{C,k,l}} = \frac{|\{x \in X_k : S_{C,k,l}(x) > 0\}|}{|X_k|}$$

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You can use $TCAV_Q$ to detect biases in datasets. For example, if you're classifying sports, you could create concepts like "man" and "woman" and calculate $TCAV_Q$ for the entire dataset. The resulting score will help you see if there is a bias in the data.

Relative TCAV

What if there are correlation between the concepts, e.g. brown hair vs. black hair, in that case $v_{C_1}^l, v_{C_2}^l$ are far from orthogonal.

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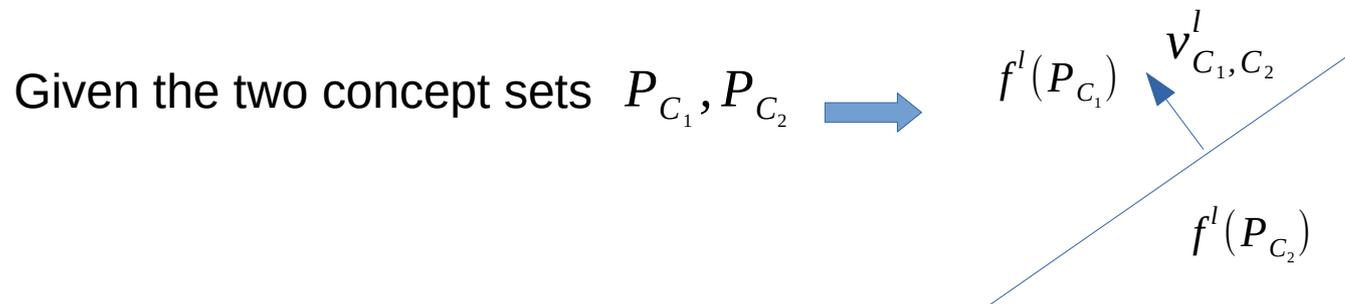
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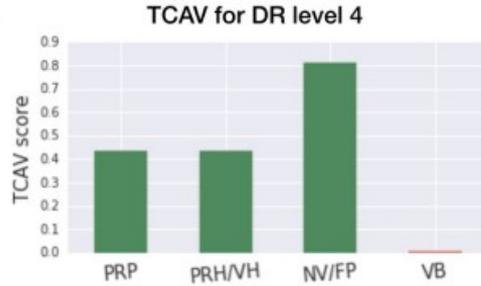
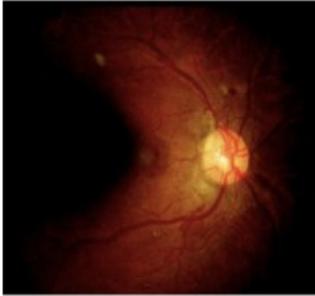
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Use previous projection but with v_{C_1, C_2}^l

Results

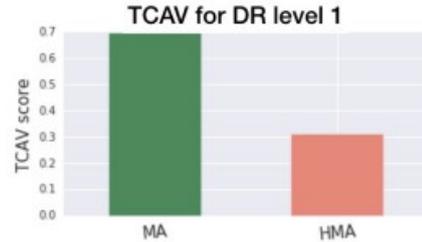
DR level 4 Retina



Diabetic Retinopathy (DR) data.

The model of interest predicts DR level using a 5-point grading scale based on complex criteria, from level 0 (no DR) to 4 (proliferative) .

DR level 1 Retina

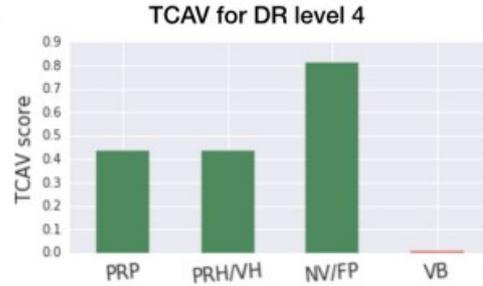
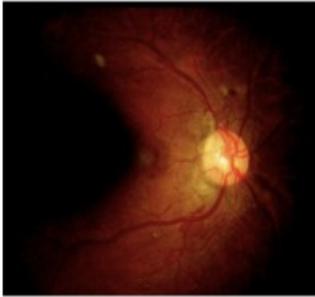


HMA distribution on predicted DR

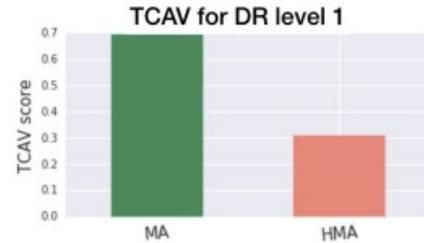


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For level 4 the model performance is good and the concepts (histogram) are in agreement with the expert expectations.

For level 1 the model performance is not so good and there is a missclassification of level 1 by level 2. The concept MA is also more relevant to level 2 so the concept is also wrong as expected,

Pros:

- 1 – Machine learning expertise not needed to employ TCAV
- 2 – Allow users to investigate any concept defined by a concept dataset.
- 3 – Provide global explanations, linking concepts to any class.
- 4 – Could help to identify potential issues or biases in model training: e.g. if a classifier is more sensitive to the concept “man” rather than “woman” it could suggest an imbalanced dataset.

Cons:

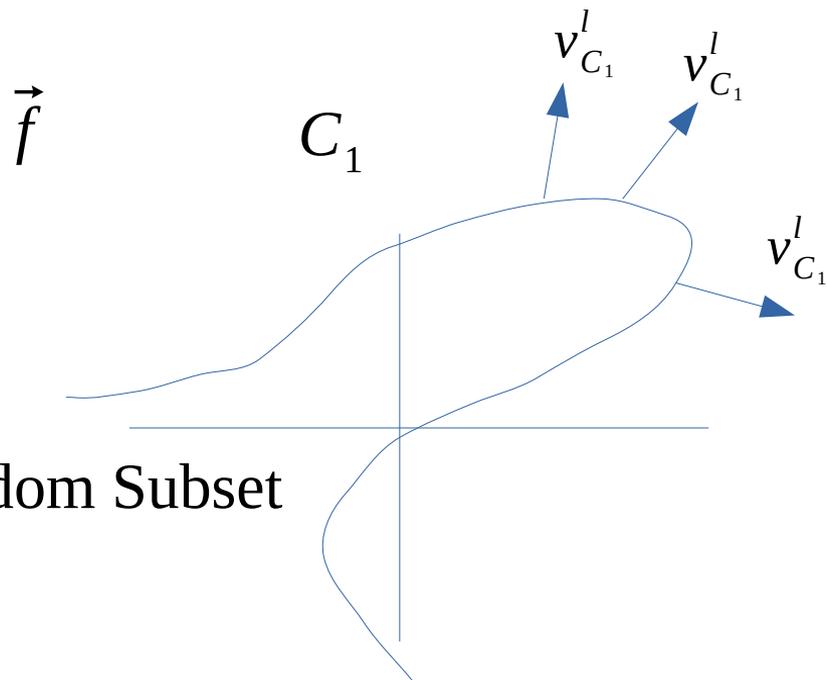
- 1 – Requires additional data for concept datasets, so it can be quite expensive.
- 2 – TCAV less applicable in shallow networks: deeper layers tend to offer better separability of concepts.
- 3 - Challenge with abstract or general concepts, e.g. "happiness". On those cases a fair amount of data is needed to train a Concept Activation Vector (CAV).

Some thoughts:

1 – TCAV only uses the sign of the sensitivity: why not the magnitude of the projection too?

2 – Why a linear classifier? Can we tackle the problem with a non-linear one?

In this case you could take into account the correlations between different concepts.



Random Subset

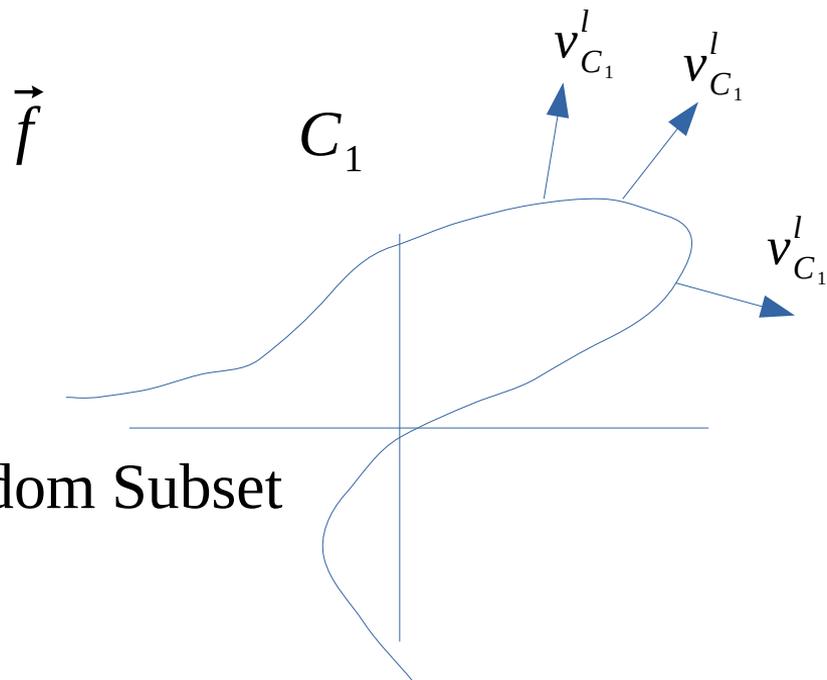
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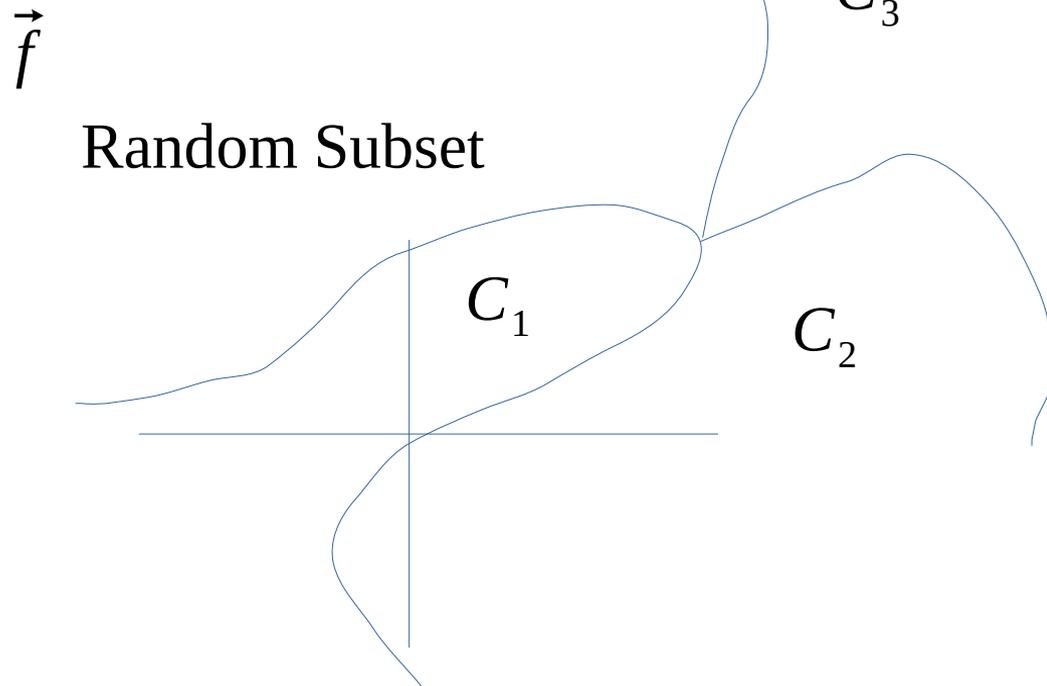
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Non-linear classifier with overlapping concepts

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One of the main differences (and **disadvantages**) with TCAV is is the **requirement for concept annotation**.

Let's give an overview to the main idea

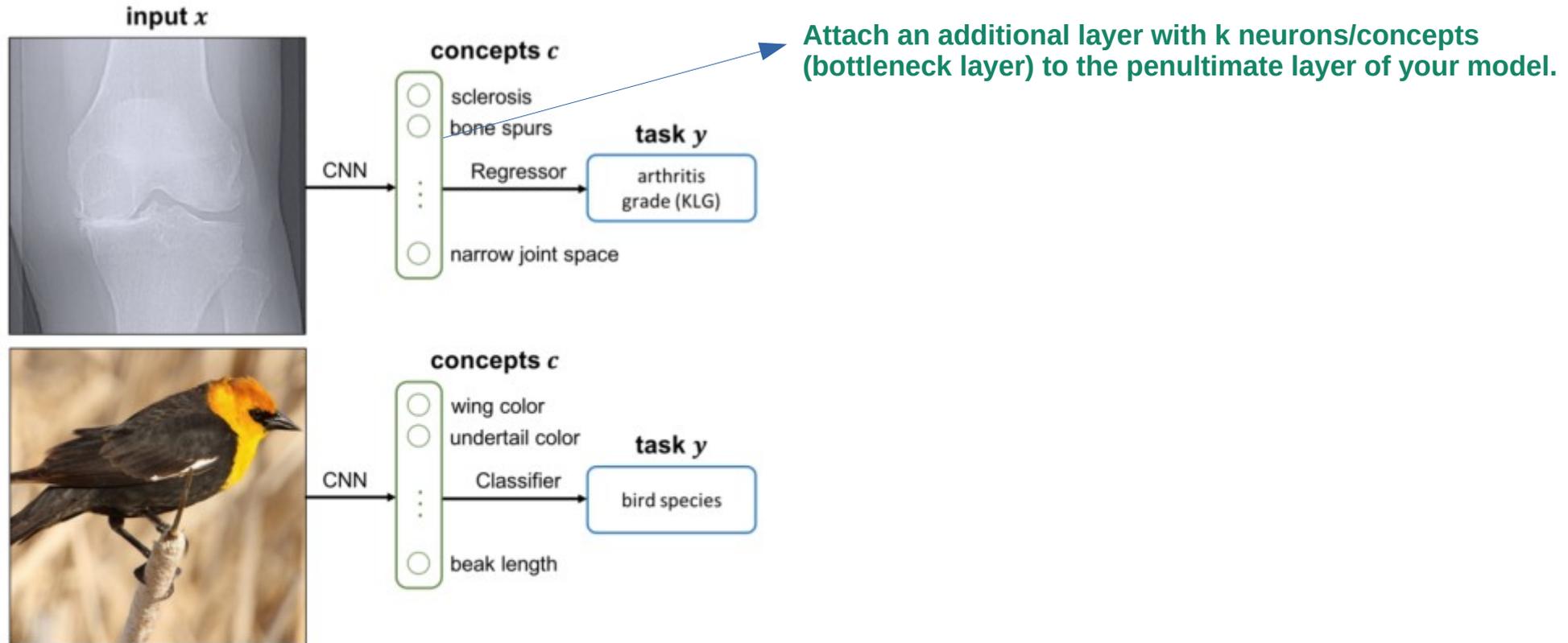
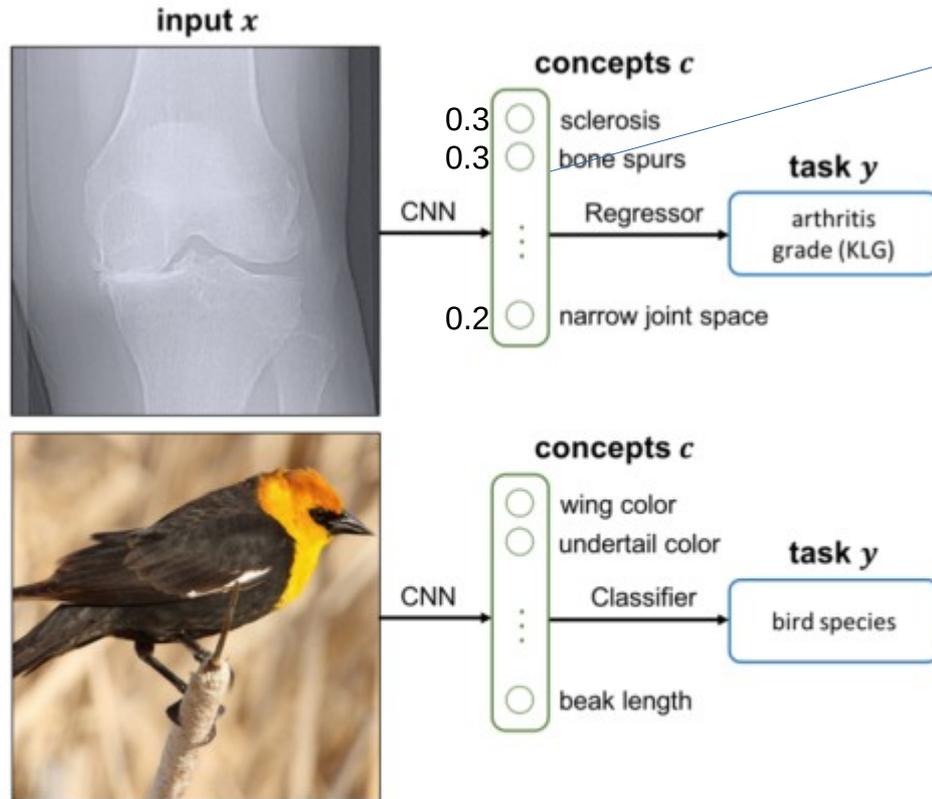


Figure 1. We study concept bottleneck models that first predict an intermediate set of human-specified concepts c , then use c to predict the final output y . We illustrate the two applications we consider: knee x-ray grading and bird identification.

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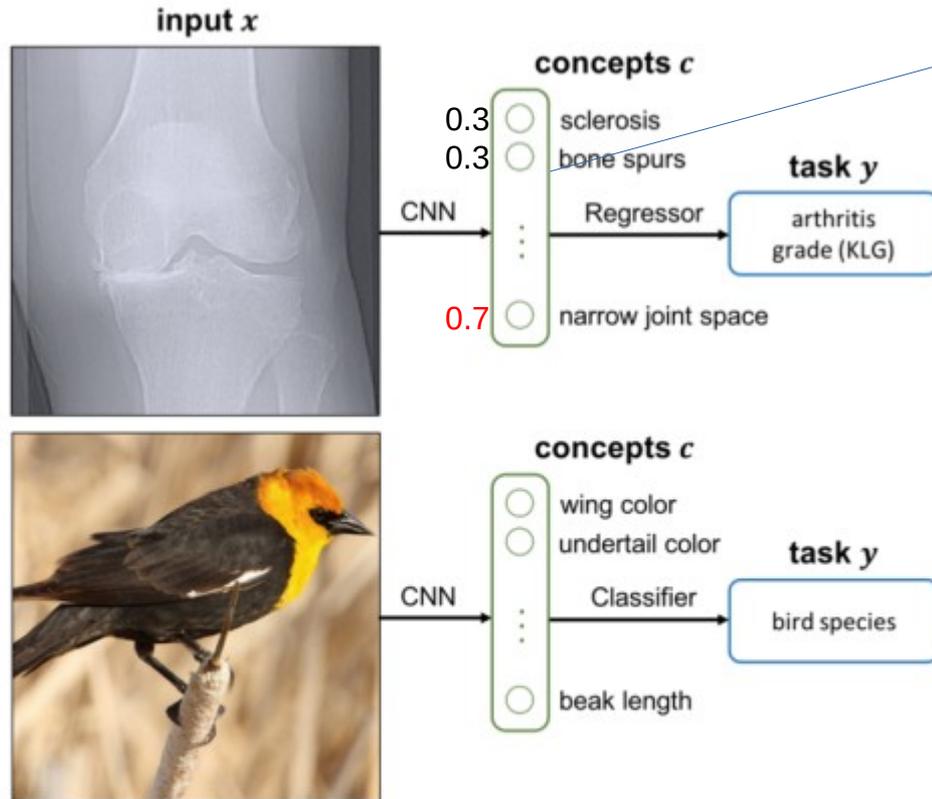


Attach an additional layer with k neurons/concepts (bottleneck layer) to the penultimate layer of your model.

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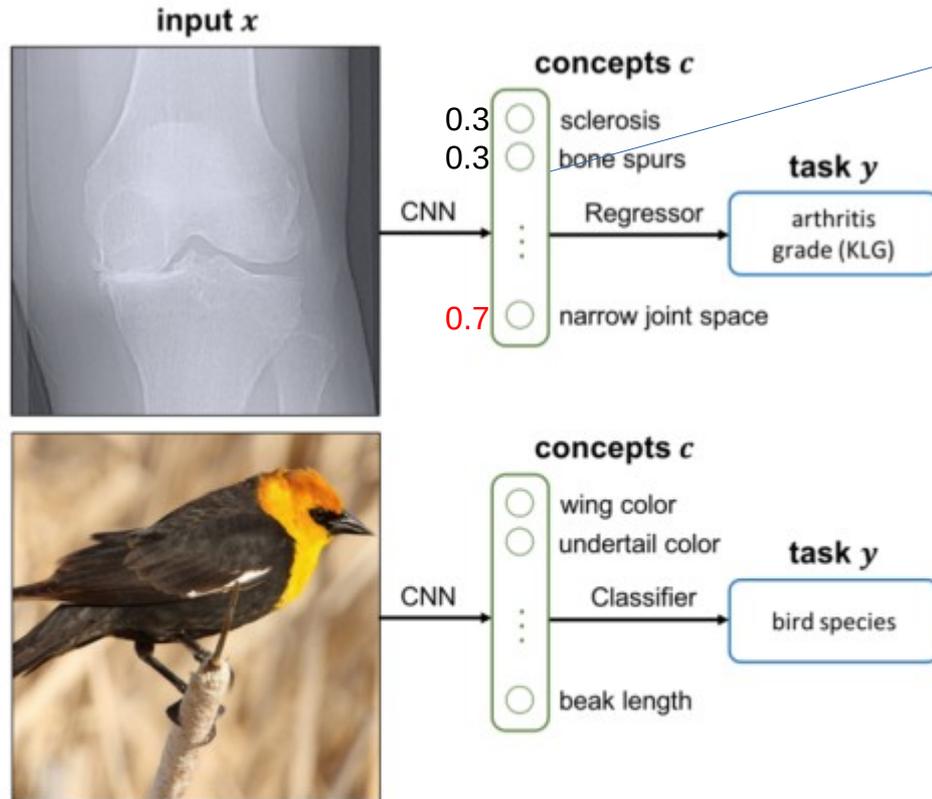


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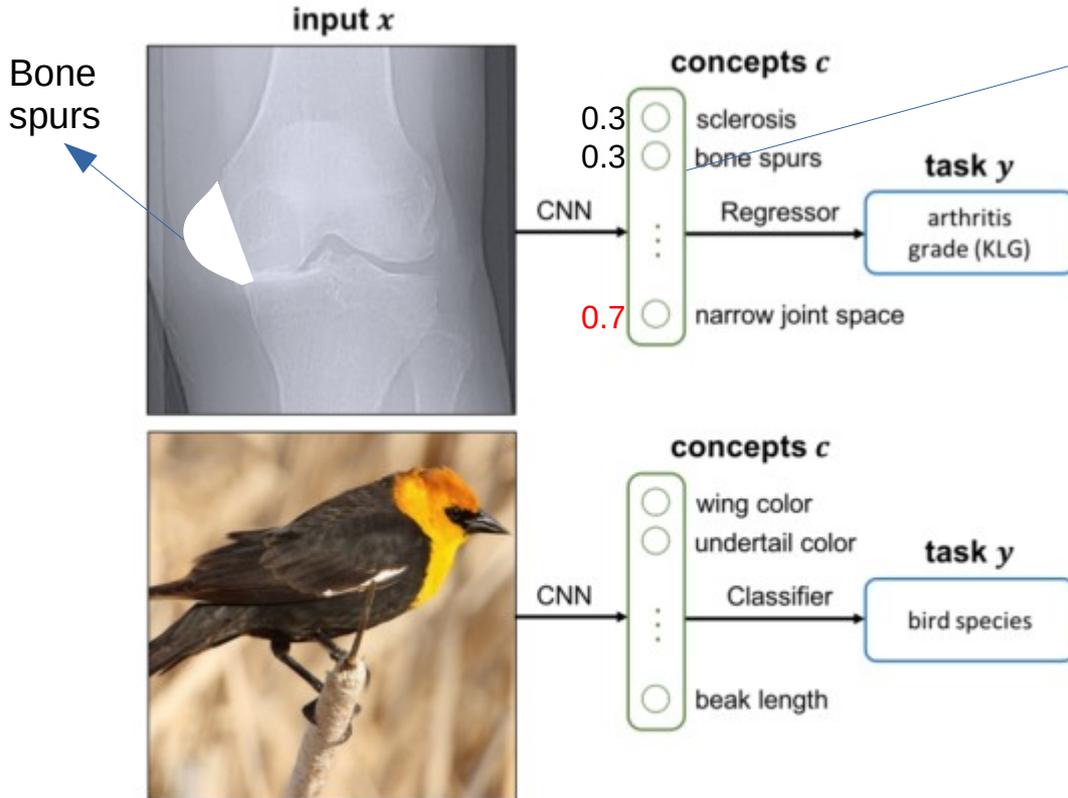
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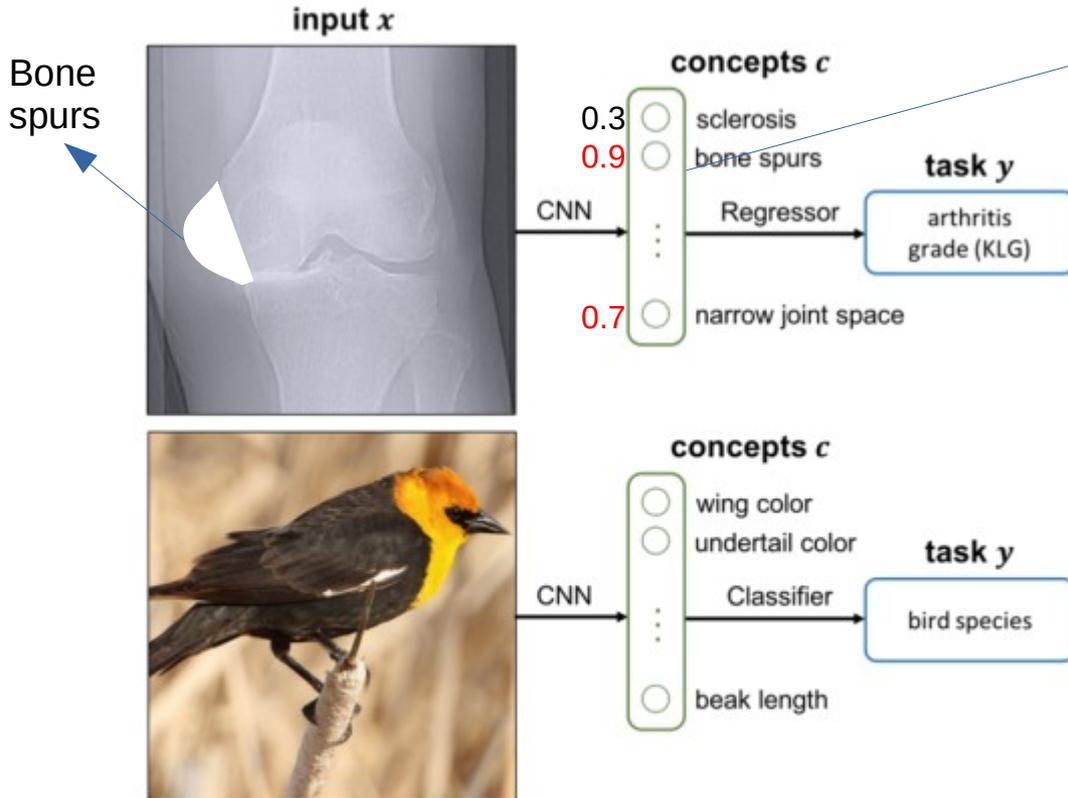
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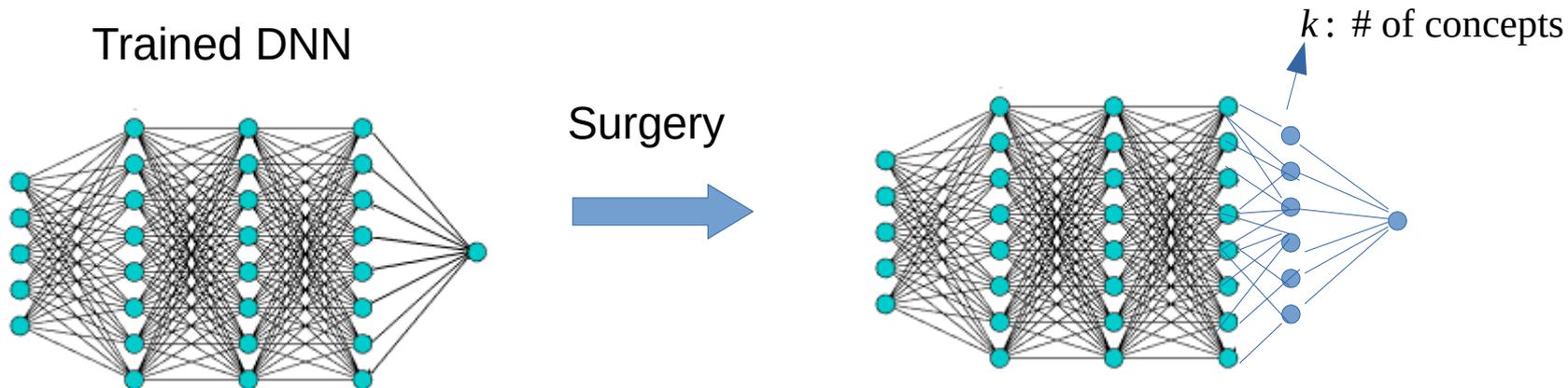
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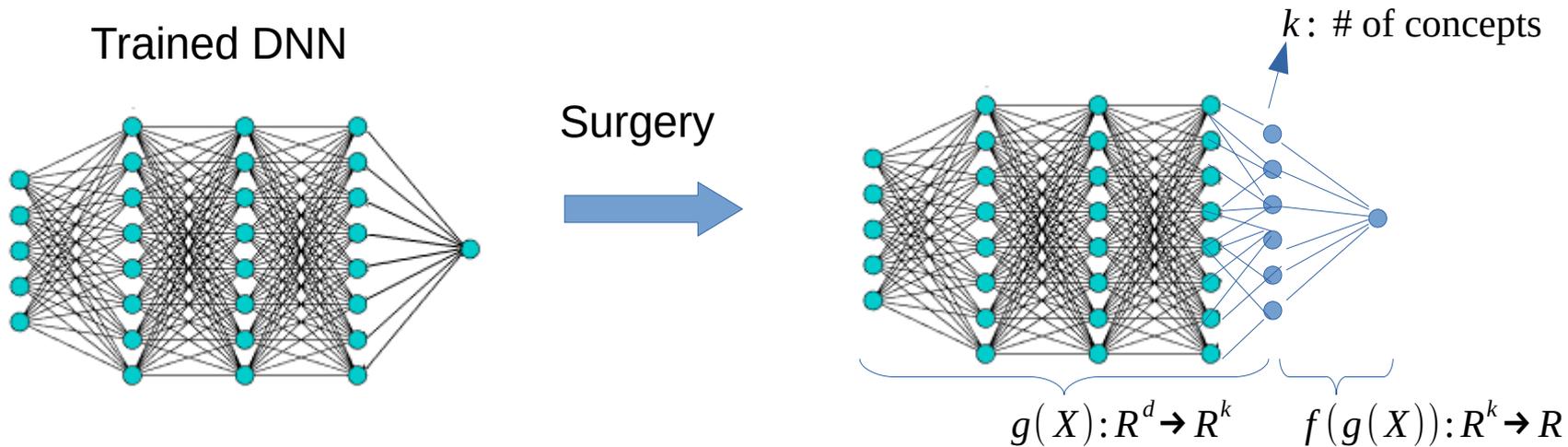
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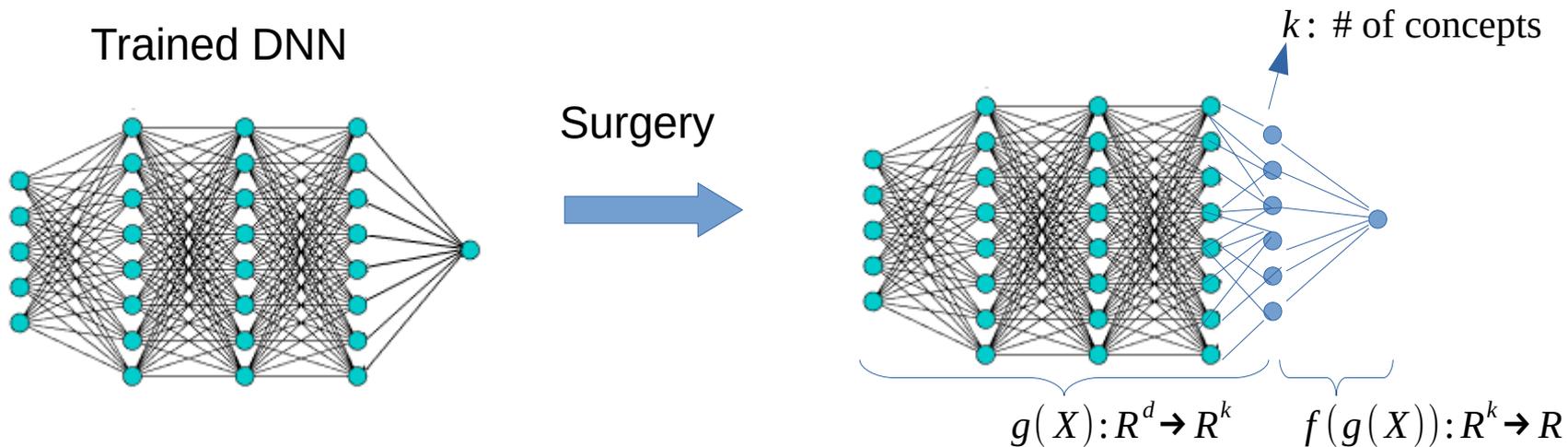
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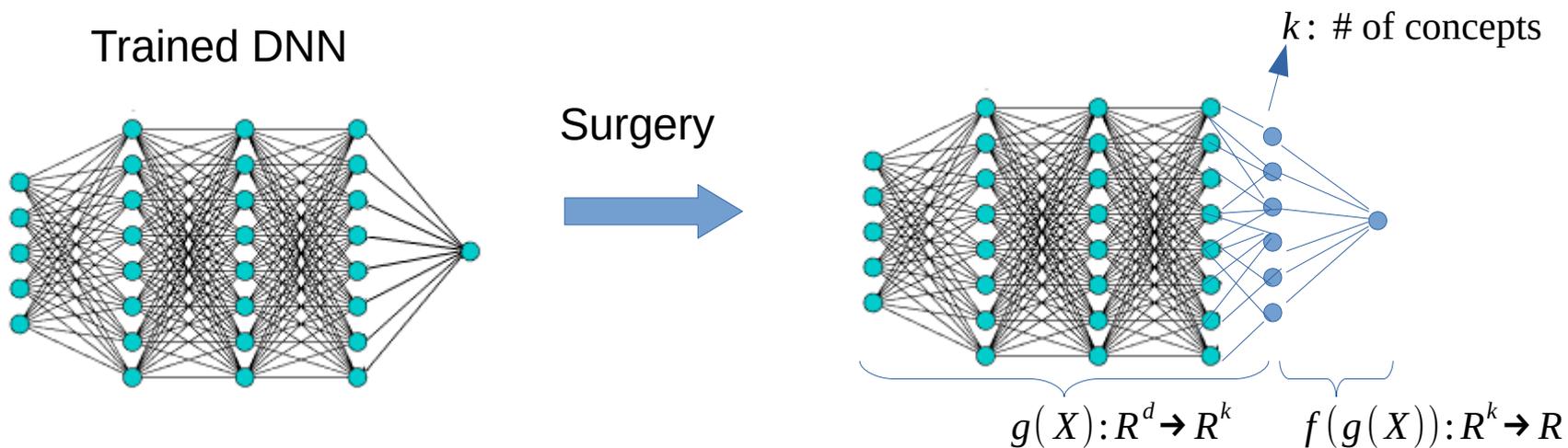


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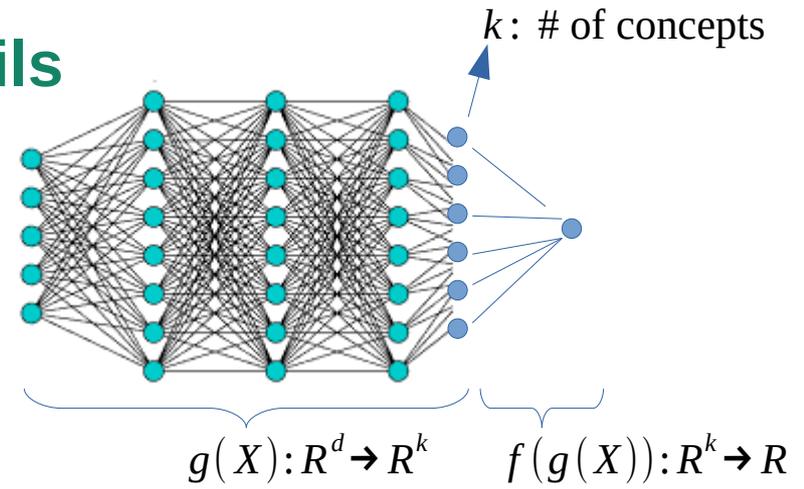
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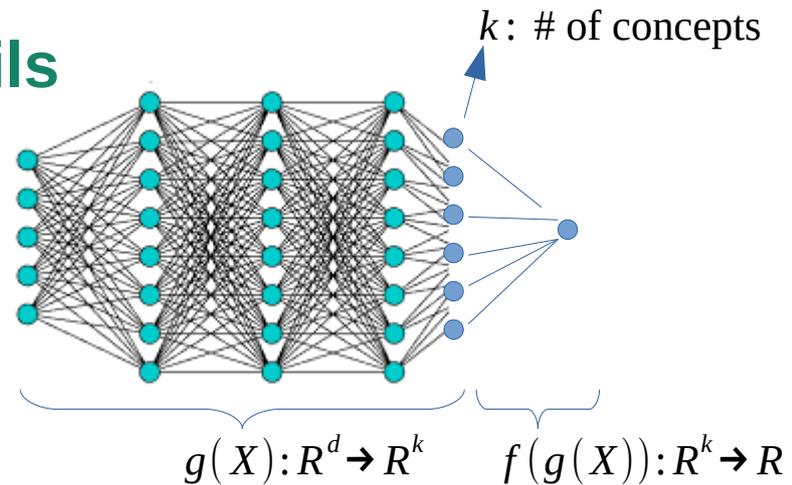
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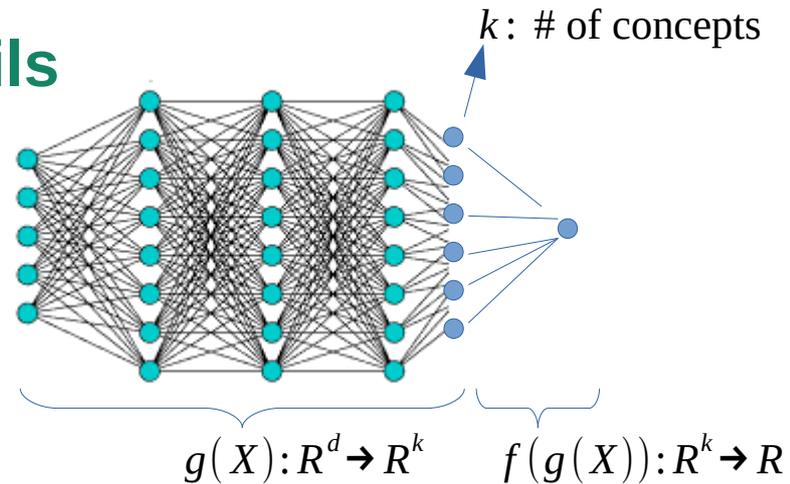
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2. **The sequential bottleneck** first learns \hat{g} in the same way as above. It then uses the concept predictions \hat{g} to learn:

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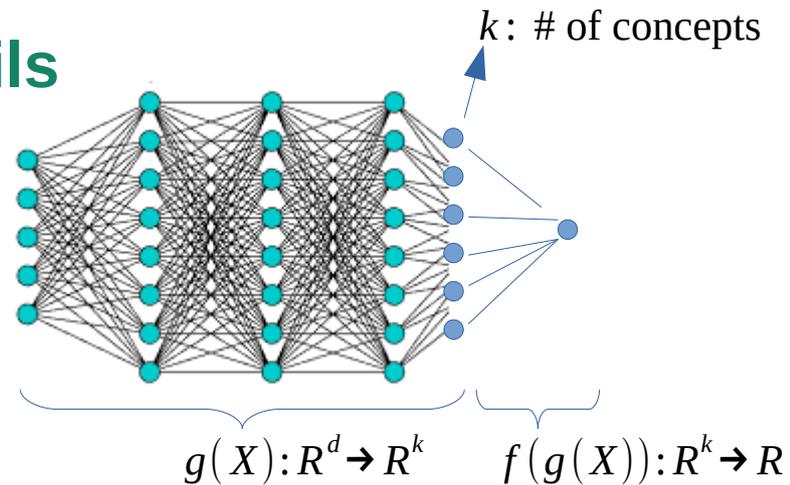
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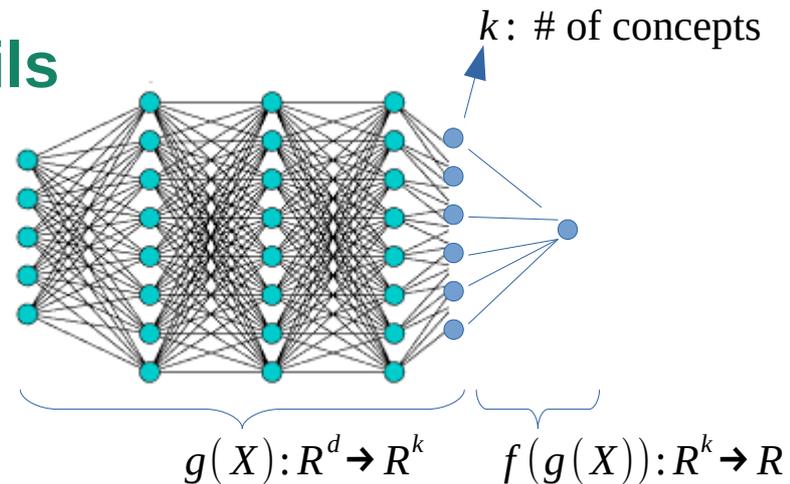
2. **The sequential bottleneck** first learns \hat{g} in the same way as above. It then uses the concept predictions \hat{g} to learn:

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3. **Standard model** (useful for benchmarking): $f, \hat{g} = \operatorname{argmin}_{f,g} \sum_i L_Y(f(g(x^{(i)}), y^{(i)}))$



Implementation details



4 – Design the cost functions for retraining the model.

The paper proposes three approaches:

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4. **The joint bottleneck** minimizes the weighted sum: $(\hat{f}, \hat{g}) = \operatorname{argmin}_{f,g} \sum_i L_Y(f(g(x^{(i)})), y^{(i)}) + \sum_j \lambda L_{C_j}(g(x^{(i)}), c_j^{(i)})$

Note that in point-3 the limit $\lambda \rightarrow \infty$ will produce the sequential bottleneck model and the limit $\lambda \rightarrow 0$ will recover the standard model.

Results

The paper works with two datasets:

X-ray grading, Osteoarthritis Initiative (OAI): Kellgren-Lawrence grade (KLG), a 4-level ordinal variable assessed by radiologists that measures the severity of osteoarthritis. Number of concepts, $k=10$. $n \sim 36K$

Bird identification (CUB): The target are 200 different bird species. Number of concepts $k=112$ binary bird attributes like wing color, beak shape, etc.

Models used: Resnet-18 (OAI) and inception-v3 (CUB)

Results

Remember, Joint model:

$$(\hat{f}, \hat{g}) = \operatorname{argmin}_{f, g} \sum_i L_Y(f(g(x^{(i)})), y^{(i)}) + \sum_j \lambda L_{C_j}(g(x^{(i)}), c_j^{(i)})$$

Target error

MODEL	y RMSE (OAI)	y ERROR (CUB)
INDEPENDENT	0.435 ± 0.024	0.240 ± 0.012
SEQUENTIAL	0.418 ± 0.004	0.243 ± 0.006
JOINT	0.418 ± 0.004	0.199 ± 0.006
STANDARD	0.441 ± 0.006	0.175 ± 0.008
NO BOTTLENECK	0.443 ± 0.008	0.173 ± 0.003

From the three proposed models, the Joint, is the best one!

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Concept error

MODEL	c RMSE (OAI)	c ERROR (CUB)
INDEPENDENT	0.529 ± 0.004	0.034 ± 0.002
SEQUENTIAL	0.527 ± 0.004	0.034 ± 0.002
JOINT	0.543 ± 0.014	0.031 ± 0.000

The accuracy on CUB is quite high ~ 97% .

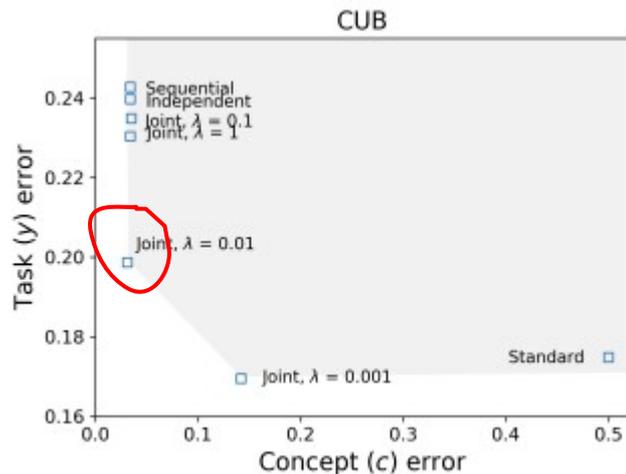
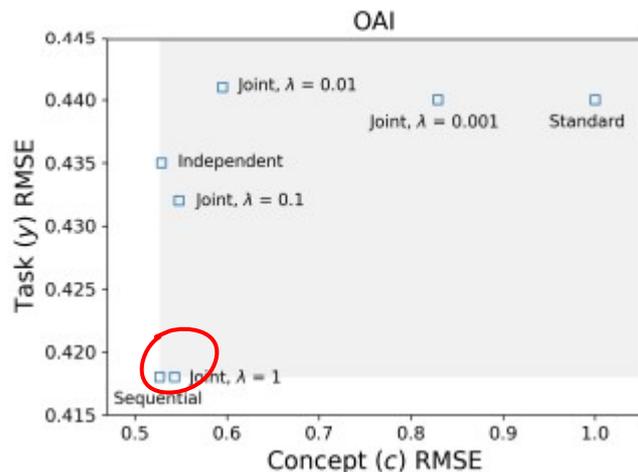
This should be the case in practice; otherwise, relying on concepts wouldn't be beneficial.

Results

$$(\hat{f}, \hat{g}) = \operatorname{argmin}_{f, g} \sum_i L_Y(f(g(x^{(i)})), y^{(i)}) + \sum_j \lambda L_{C_j}(g(x^{(i)}), c_j^{(i)})$$

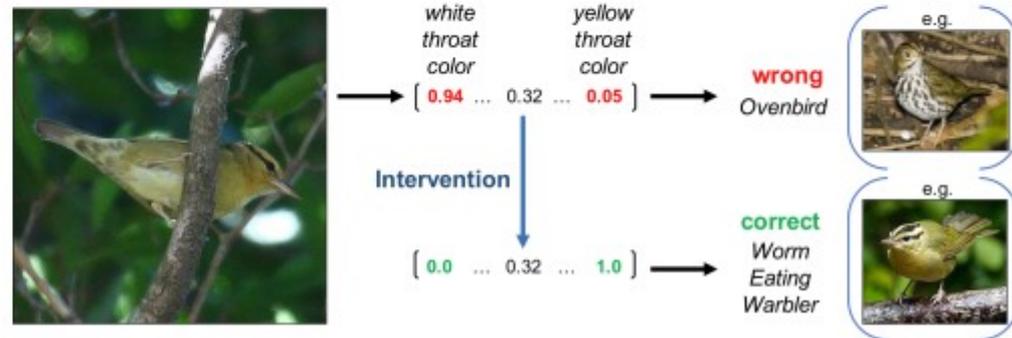
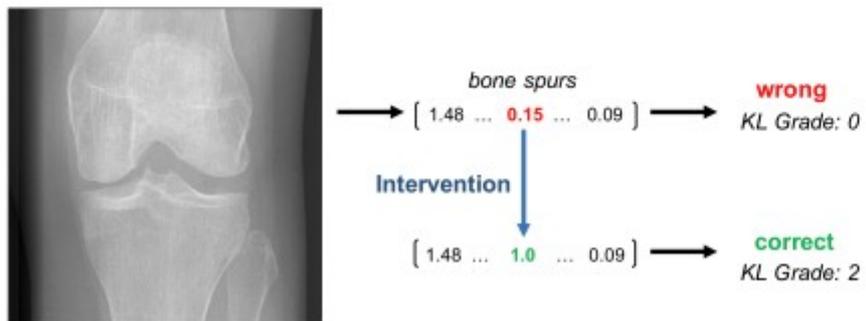
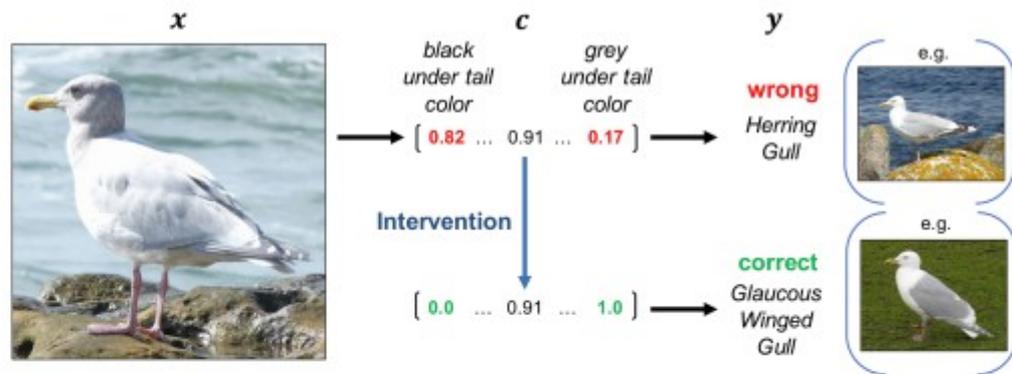
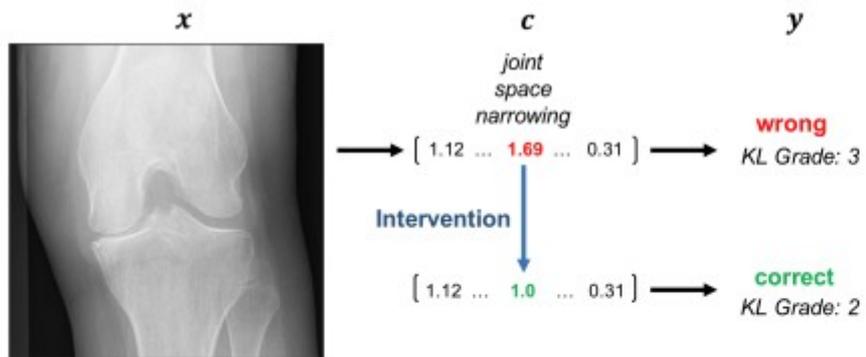
The points in red are the ones we are interested in, as we aim for the highest possible concept accuracy while maintaining good task accuracy.

In general, the joint model is performing better, as expected!



Results

Concept Intervention



General questions:

- 1 - If the bottleneck is not very representative, could the model's performance decrease?
- 2 - In the case of osteoarthritis, where concepts are highly correlated with the target, does the model find it easier to understand them?
- 3 - When conducting concept intervention with 100 concepts, how should you proceed? How do you determine which concepts to adjust, and what are the appropriate values?

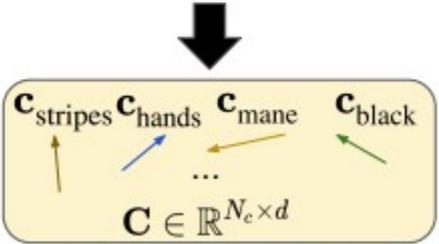
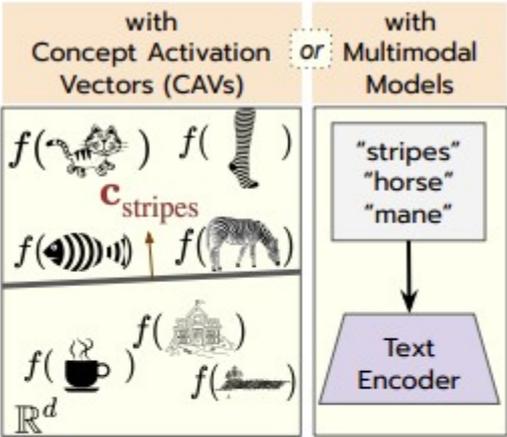
Post-hoc CBM (PCBM)

Combining the strengths of TCAV and CBM, it offers an easy way to create concepts similar to TCAV (even simpler) while providing the ability to interact with them as in CBM.

PCBM idea

CAV generation:

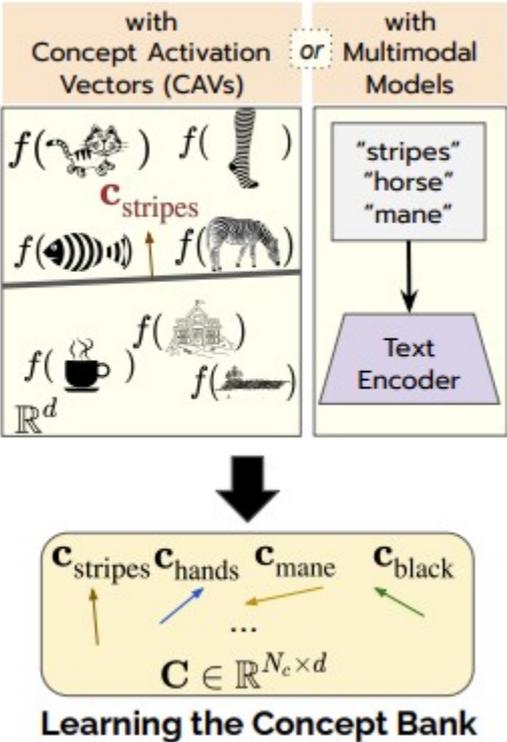
A – TCAV approach



Learning the Concept Bank

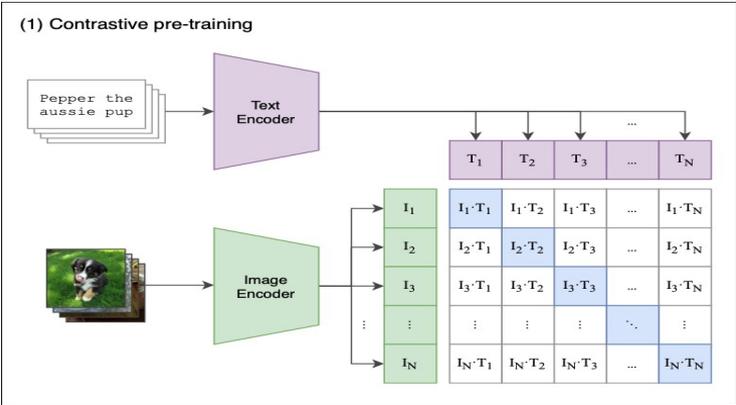
PCBM idea

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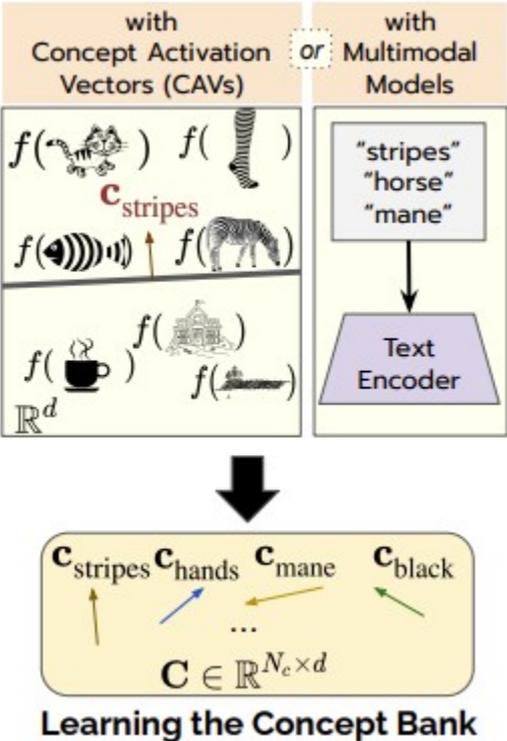
A – TCAV approach

B – Multimodal Models (Image/Test like CLIP)



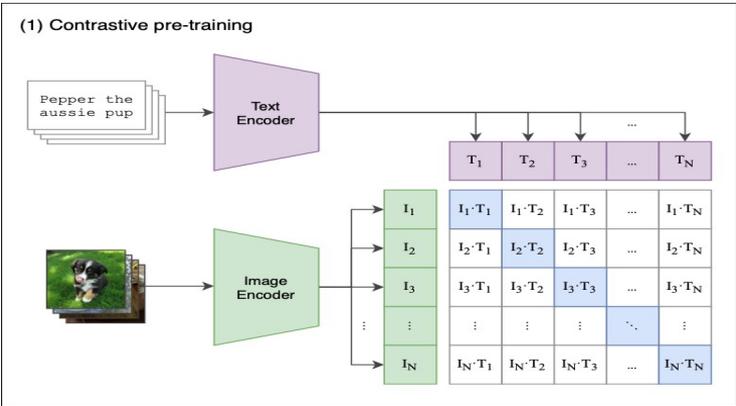
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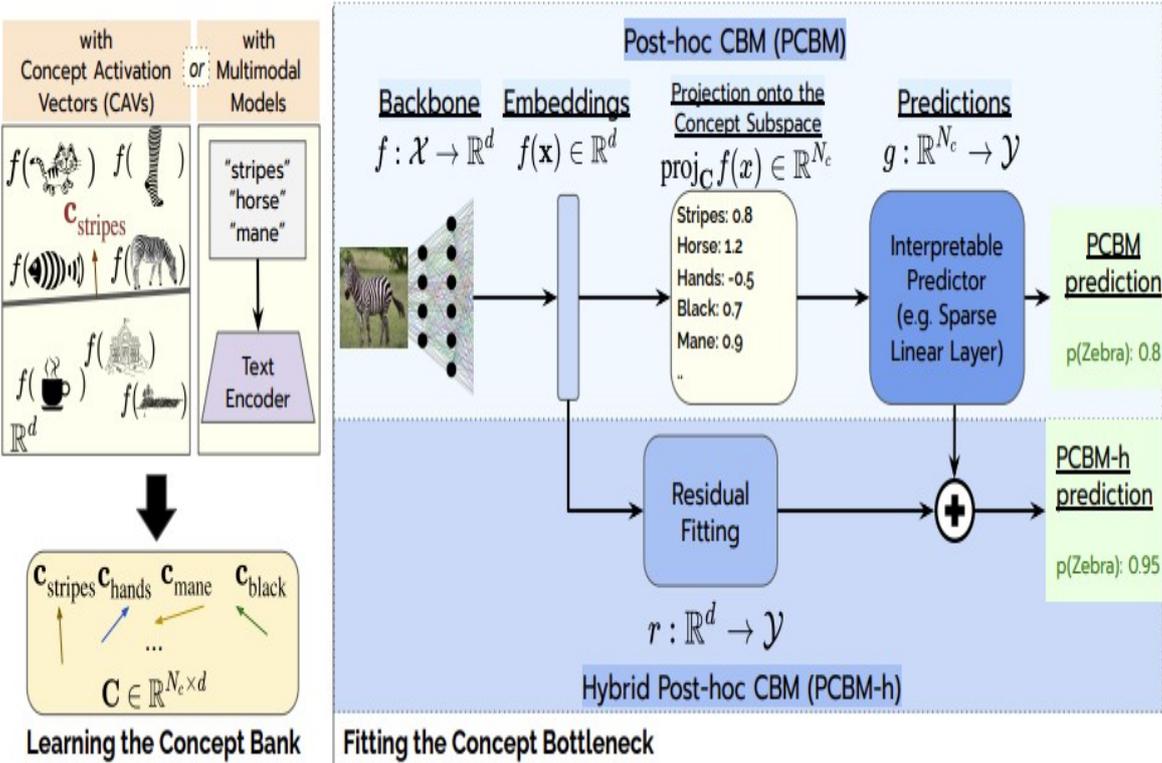


Q. We cannot expect TCAV and CLIP embedding to be similar, right?. However there is a retraining process ...

PCBM idea

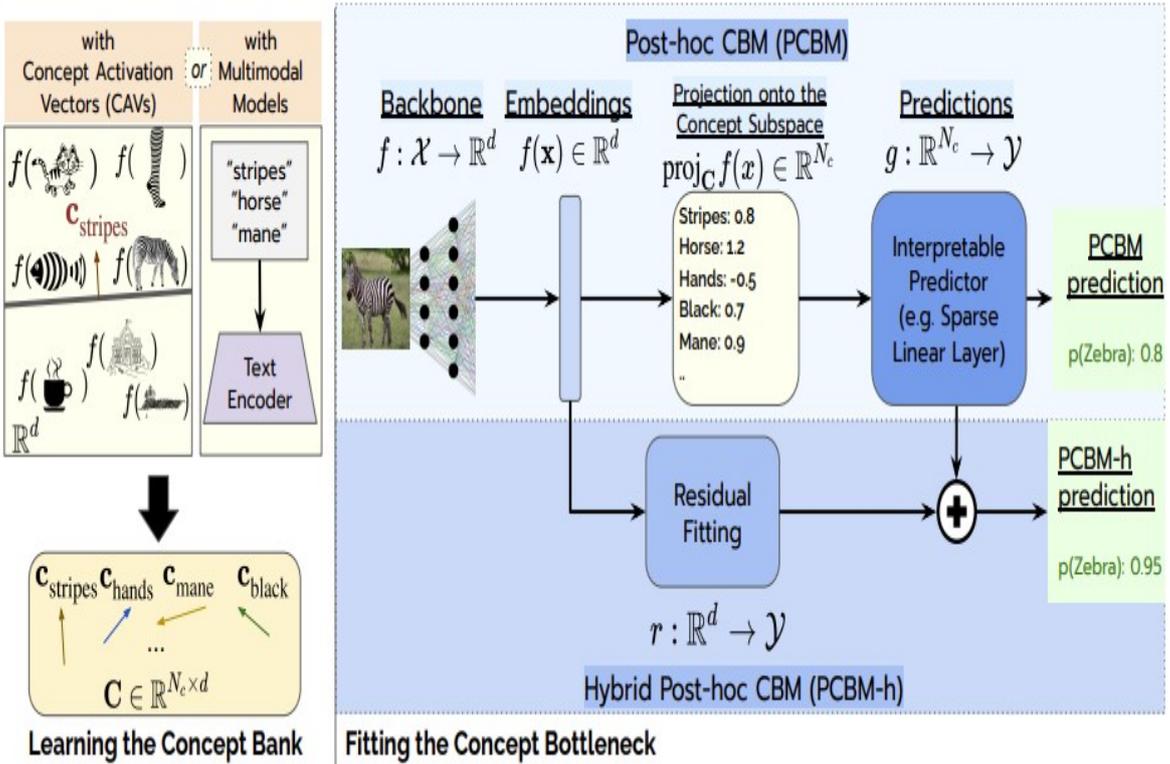
1 – Learning the concept bank

PCBM architecture:



PCBM idea

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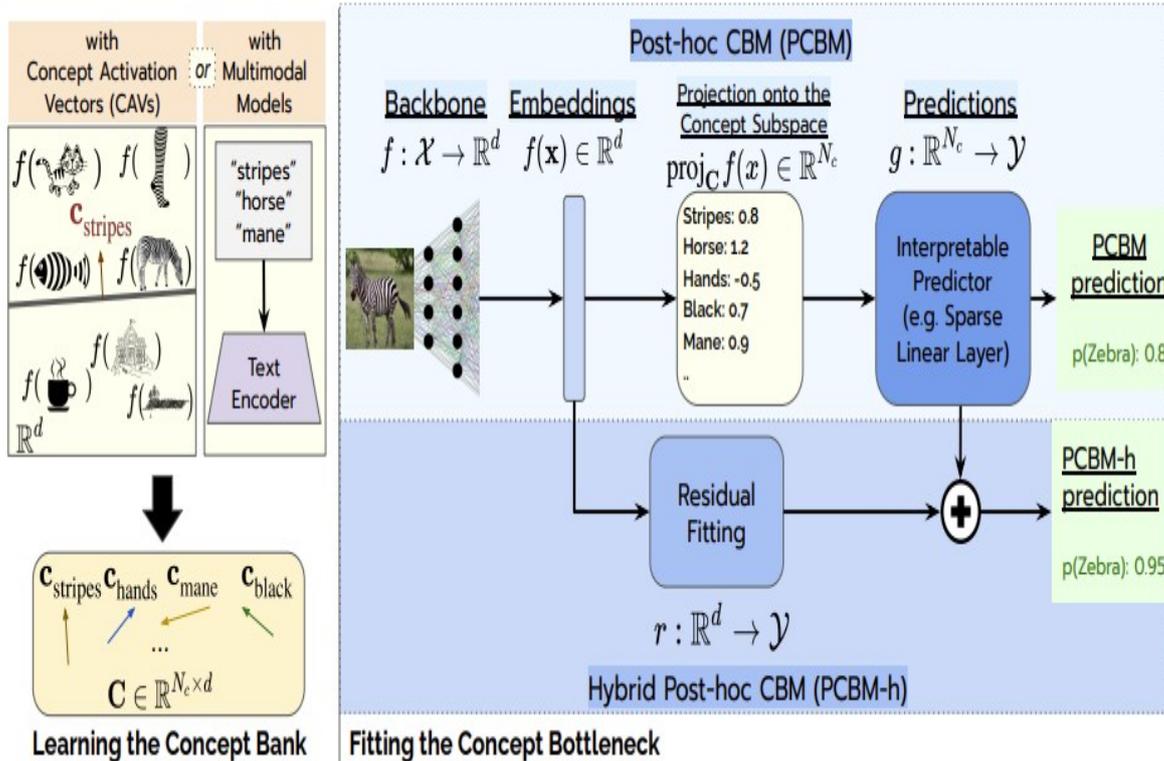


1 – Learning the concept bank

2 – **Backbone model:** This is your trained DNN with the penultimate layer attached to the embedding $f(X)$ (similar to what we did in CBM).

PCBM idea

PCBM architecture:



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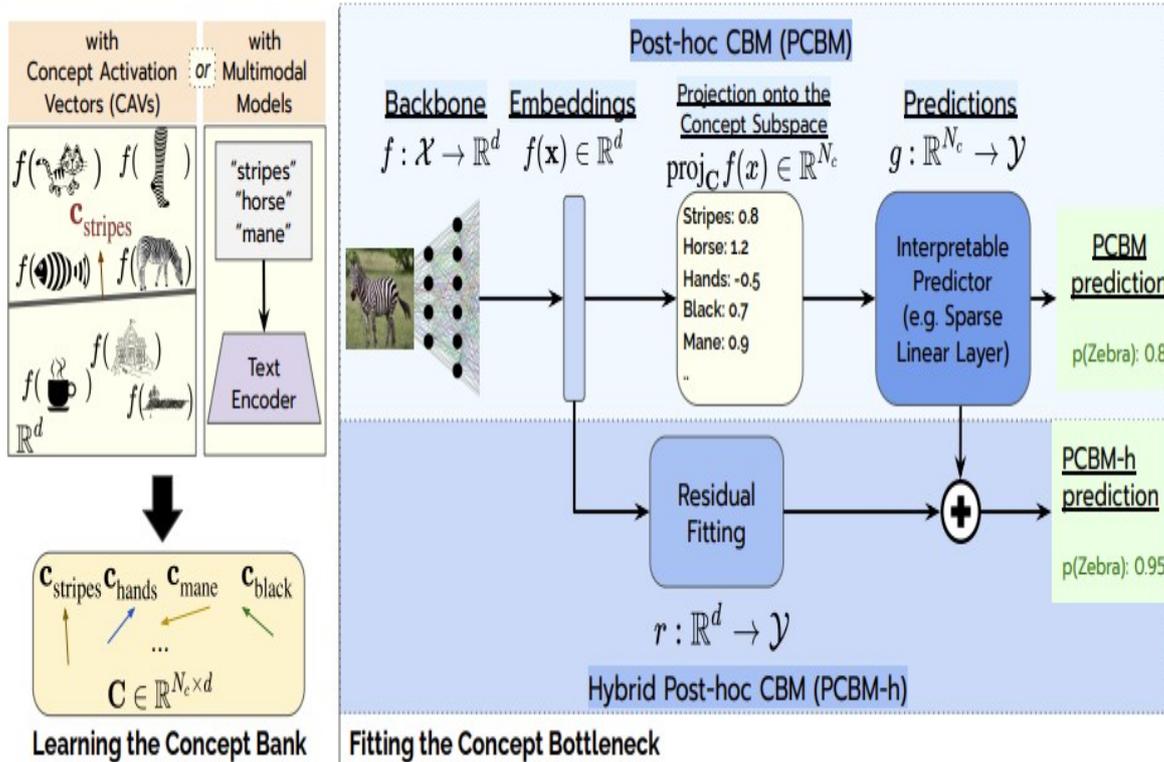
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3 – Projection into concept subspace.

$$\text{proj}_C f^{(i)}(X) = \frac{\langle f(x), c_i \rangle}{\|c_i\|^2} \quad \text{with } i=1, \dots, N_C$$

PCBM idea

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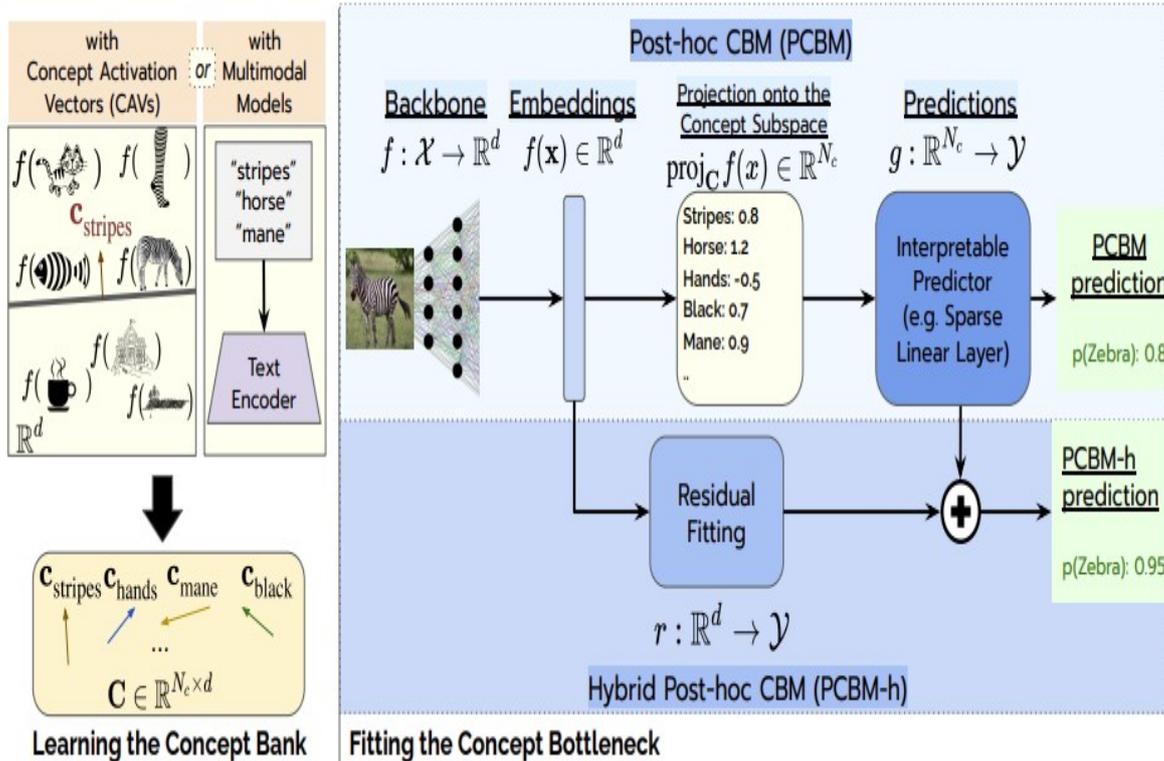
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$$g: \mathbb{R}^{N_c} \rightarrow \mathcal{Y}$$

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5 – **Residual Fitting:** If prediction space is not representative enough we could have a decrease in original's model performance.

Residual Fitting Module: focuses in accuracy rather than concepts.

The model with the residual module is call hybrid PCBM (PCBMh)

Experiments

PCBMs achieve comparable performance to the original model

	CIFAR10	CIFAR100	COCO-Stuff	CUB	HAM10000	ISIC
Original Model	0.888	0.701	0.770	0.612	0.963	0.821
PCBM	0.777 ± 0.003	0.520 ± 0.005	0.741 ± 0.002	0.588 ± 0.008	0.947 ± 0.001	0.736 ± 0.012
PCBM-h	0.871 ± 0.001	0.680 ± 0.001	0.768 ± 0.01	0.610 ± 0.010	0.962 ± 0.002	0.801 ± 0.056

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Observations:

PCBMs match the performance of the original model in HAM10000 and ISIC, with as few as 8 human-interpretable concepts

In CIFAR100, it seems that the concept bank available is not sufficient to classify finer-grained classes

The residual component of PCBMh only intervenes when the prediction is wrong and fixes the mistake. In general this happened when the concept bank is not sufficiently expressive.

Experiments

PCBM using CLIP concepts:

	CIFAR10	CIFAR100	COCO-Stuff
Original Model (CLIP)	0.888	0.701	0.770
PCBM & labeled concepts	0.777 ± 0.003	0.520 ± 0.005	0.741 ± 0.002
PCBM & CLIP concepts	0.833 ± 0.003	0.600 ± 0.003	0.755 ± 0.001
PCBM-h & CLIP concepts	0.874 ± 0.001	0.691 ± 0.006	0.769 ± 0.001

of CLIP concepts: 206 527 822

Observations:

The original model is CLIP so $f(X)$ resides in the same encoding space as the CAVs. It will be nice to see what happens with a different 'Original Model'.

If the concept space is too large how do you interact with it?

Experiments

Human concept intervention

Use a test dataset with a distributional shift: e.g. training dataset includes the class 'table' and test dataset includes the same class "table" but always with a dog.

Some concepts may be irrelevant for prediction due to the distributional shift. How do we select the relevant ones?

Experiment: Participants are given a set of concepts and asked to decide which ones should be pruned for improved accuracy, considering the importance of each concept for that class.

Conclusion: Humans are generally effective at selecting useful concepts that improve accuracy in most cases.

Conclusions

- The notion of high-level concepts is appealing and can be beneficial in real applications.
- A method like PCBM, which combines the strengths of both TCAV and CBM, and offers the flexibility to incorporate CAVs from multi-modal models, has the potential to be a game-changer for concept-based interpretable Neural Networks.
- However, it still appears impractical because the concept spaces are too large. Nonetheless, as demonstrated in the PCBM paper, human intervention can help reduce the concept space while maintaining accuracy but the evidence is not conclusive to be used in practice.
- Another issue is that multimodal models may struggle to generate accurate CAVs in highly specialized fields.

Thank you !!!