Concept-based Models

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Advanced Topics in Machine Learning & Optimization — 2023-24

The State of XAI

- **White-box models**:
  - Shallow decision trees, sparse linear models, rule lists, . . .
  - Explanations for free
  - Well suited for, e.g., tabular data
  - Low performance on non-tabular data, specifically because they don't support representation learning.

- **Black-box models** + **post-hoc explainers**:
  - Like neural nets + LIME, SHAP, Input Grads
  - High performance on non-tabular data like images and text thanks to representation learning.
  - Perturbation-based explanations are expensive to compute and can have high variance
  - Gradient-based explanations are widely applicable and cheap to compute, but they are often too "local".

Tree Regularization

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Idea: take a black-box f_θ and make it "more interpretable":

- If f_θ is a dense linear model, add a sparsifying L_1 regularizer so that its weight vector contains many zeros.
- This makes the model more *simulatable*: "take in input data together with the parameters of the model and in reasonable time step through every calculation required to produce a prediction" Lipton (2018)

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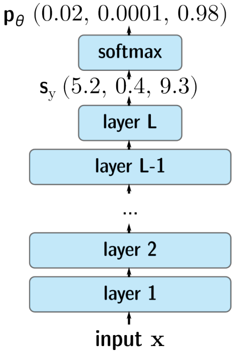
- Can we make a neural network **behave like a decision tree** – so as to facilitate conversion into one using, e.g., LIME? **Yes** Wu et al. (2018)

- Take a regular neural network $p_\theta(y \mid \mathrm{x})$ and a training set $S = \{(\mathrm{x}_i, y_i) : i = 1, \ldots, m\}$. Normally, you would train it by minimizing the following empirical loss:

$$\frac{1}{|S|} \sum_{(\mathrm{x},y)\in S} -\log p_\theta(\mathrm{x}, y)$$



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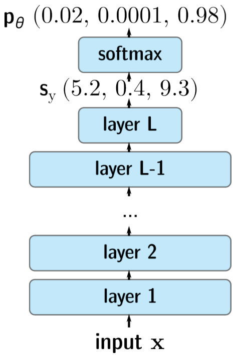
$$\frac{1}{|S|} \sum_{(\mathrm{x},y)\in S} \left(-\log p_\theta(\mathrm{x}, y) + \lambda \cdot \Omega(\theta, \mathrm{x}) \right)$$

where $\Omega(\theta, \mathrm{x})$ is the **average depth** of a shallow DT that fits f_θ in the neighborhood of x



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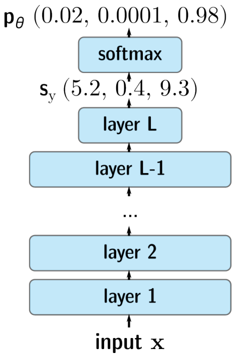
- Ω is small only if $f_\theta(\mathrm{x})$ can be simulated locally by a small DT



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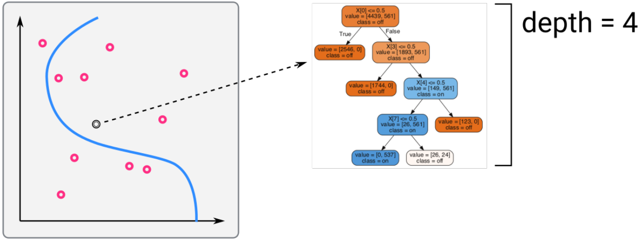

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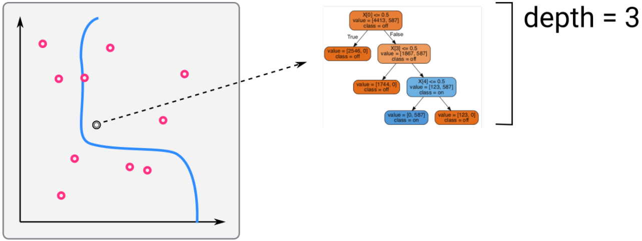

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Idea: learn an **auxiliary regressor** $d_\mu(\theta, \mathbf{x})$ that, given $\mathbf{x}$, **predicts the average depth of a DT** that fits f_θ **from the parameters** θ themselves

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  - Update θ by performing one *epoch* of gradient descent on the modified loss:

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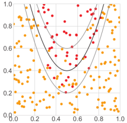
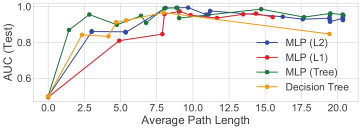
- Under the assumption that θ doesn't change "too much" across epochs, one can warm start training μ from the previous epoch.

Example: Fitting a Parabola

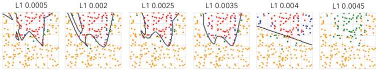


(a) Training Data and Binary Class Labels for 2D Parabola

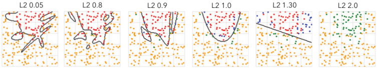


(b) Prediction quality and complexity as reg. strength λ varies

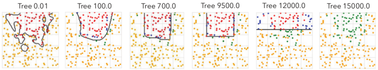
- For $\lambda = 9500$ (the exact value is not important) the tree-regularized network recovers exactly the shape of a **DT with depth** 2. Increasing λ further further flattens the tree to depth 1, at the cost of accuracy.



(c) Decision Boundaries with L1 regularization



(d) Decision Boundaries with L2 regularization



(e) Decision Boundaries Tree regularization

Figure 2: *2D Parabola task*: *(a)* Each training data point in 2D space, overlaid with true parabolic class boundary. *(b)*: Each method's prediction quality (AUC) and complexity (path length) metrics, across range of regularization strength λ. In the small path length regime between 0 and 5, tree regularization produces models with higher AUC than L1 or L2. *(c-e)*: Decision boundaries (black lines) have qualitatively different shapes for different regularization schemes, as regularization strength λ increases. We color predictions as true positive (red), true negative (yellow), false negative (green), and false positive (blue).

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Yes: change the nets' architecture

From Inputs/Examples to Concepts

- Post-hoc explainers can be **unfaithful** (Teso, 2019)

Toward Faithful Explanatory Active Learning

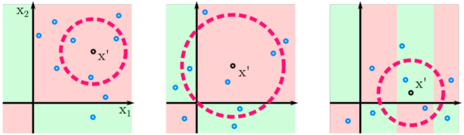


Fig. 1. Examples on which LIME produces unfaithful explanations. The decision surface of f is represented by the colored areas: light green means positive, light red negative. The pink circle represents the kernel k: points inside of it are assigned substantial weights while all others are not. Left: all synthetic examples with large weight have the same label. Middle: the synthetic examples fail to capture the non-additive interaction of the two features. Right: the kernel is too broad, and the synthetic dataset is highly complex and non-linear.

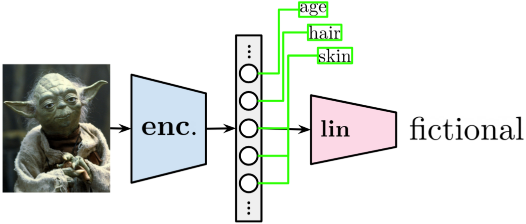
- Unfaithful explanations mean the user might be **correcting non-existent bugs!**

From Inputs/Examples to Concepts

- Low-level explanations are **ambiguous** (Rudin, 2019)

- Is it classified as “`positive`” because it is “`red`”, because it is “`sporty`”, or because it is a “`car`”?
- Human communication makes heavy use of **high-level concepts**!

Concept-based models (CBMs) are "gray-box" models [1] that support high-dimensional inputs & **representation learning** without giving up on **interpretability**.



(1) Map input to high-level **concepts** in a black-box manner

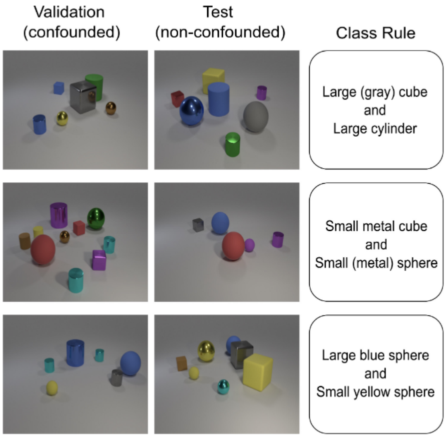
(2) Compute a prediction from the **concepts** in a white-box manner

(3) If concepts are interpretable, predictions admit **faithful** explanations like:

"`fictional`" because {**age** : -0.05, **hair** : $+0.02$, **skin** : 0.9}

The Simplest Case

- I will focus on **concepts** that are:
  - Concrete.
  - Categories: “`dog`”, “`ball`”.
  - Properties: “`red`”, “`shiny`”.
  - Atomic: no hierarchy, no real grammar.
  - Simple compositionality: “`red and shiny`”.
- This case is complicated enough already ;-)



(Source: The CLEVR-HANS data set (Stammer et al., 2021))

Concept-based Models (CBMs)

Concept-based Models

A model f_θ is **gray-box** if it combines uninterpretable black-box components with a white-box skeleton and:

- It **automatically outputs explanations** for all of its decisions
- Its explanations are **cheap** to compute
- Its explanations are **faithful** (and hence **low-variance**)
- Features **large capacity** and **representation learning**

aka "partially interpretable models" because only parts of their decision process are transparent.

- We will see different classes of CBMs:
  - Self-explainable Neural Networks (SENNs)
  - Prototype-based Networks (ProtoNets, PCNs, PPNets)
  - Concept-bottleneck Models (CBNMs)

Self-explainable Neural Networks

A **linear model** has the form:

$$f(\mathbf{x}) = \mathrm{sign}\Big(\underbrace{\sum_{i \in [d]} w_i x_i + b}_{\text{“score” of } \mathbf{x}} \Big)$$

A linear model is **sparse** if $\mathbf{w} \in \mathbb{R}^d$ few non-zero entries Tibshirani (1996); Ustun and Rudin (2016) and dense otherwise. We will briefly *forget* about sparsity for now.

It is **easy** to gather an intuitive understanding of what the model does:

- $w_i > 0 \implies x_i$ correlates with, aka “votes for”, the positive class
- $w_i < 0 \implies x_i$ anti-correlates with, aka “votes against”, the positive class
- $w_i \approx 0 \implies x_i$ is irrelevant: changing it does not affect the outcome

Example: Papayas

Does a **papaya** x taste good?

Consider a linear classifier:

$$\begin{aligned} f(\mathrm{x}) = \mathrm{sign}\big(\, & 1.3 \cdot \mathbb{1}(\mathrm{x} \text{ pulp is orange}) + \\ & 0.7 \cdot \mathbb{1}(\mathrm{x} \text{ skin is yellow}) + \\ & \mathbf{0} \cdot \mathbb{1}(\mathrm{x} \text{ is round}) + \\ & -0.5 \cdot \mathbb{1}(\mathrm{x} \text{ skin is green}) + \\ & -2.3 \cdot \mathbb{1}(\mathrm{x} \text{ is moldy}) \,\big) \end{aligned}$$

Figure 1: A bunch of papaya fruits.

It is easy to read off what attributes are "for" and "against" x being tasty **for the model** – specifically because the model encodes independence assumptions, e.g., that the shape of x is unrelated to its color.[1]

[1] When **explaining** a decision made by the model, **it is irrelevant whether these assumptions match how reality works**: we are explaining the model's reasoning process, or equivalently its interpretation of how reality works, not reality itself!

- **Linear models** only work for linear data and cannot perform representation learning: their only parameters are weights, and these are applied to the inputs directly!
- We already know that to turn a linear model work in a non-linear one it is sufficient to embed all points, giving:

$$p(1 \mid \mathbf{x}) = \sigma\Big(\sum_i w_i x_i\Big) \quad \mapsto \quad p(1 \mid \mathbf{x}) = \sigma\Big(\sum_i w_i \phi_i(\mathbf{x})\Big)$$

where, e.g., $\mathbf{x}$ are words in a document and $\phi(\mathbf{x})$ is a BERT or TF-IDF embedding. However, doing so **forfeits interpretability**!

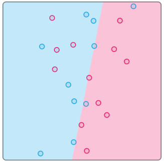
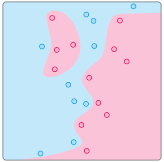


Illustration of a linear model. It cannot separate data with a complex, non-linear distribution.



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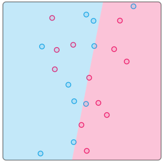

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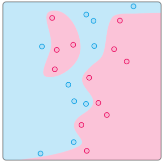

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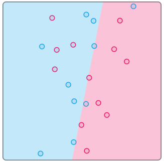
- Idea: take a non-linear model (e.g., a neural net) but ensure that it **behaves like a linear model** at any given point $\mathbf{x} \in \mathbb{R}^d$!



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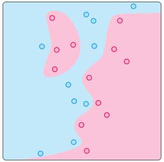

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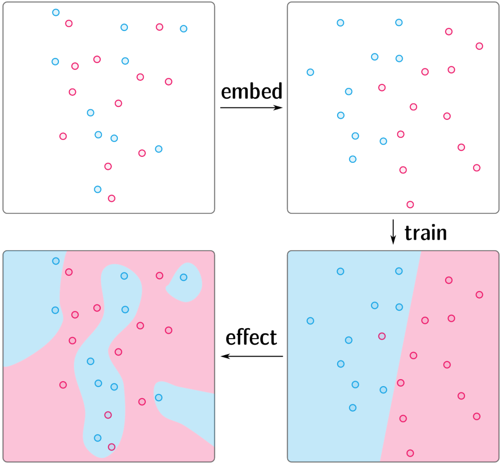
Illustration of Embedding



Top left: original data, not lineary separable. **Top right**: embedded data, now more easily seprable. **Bottom right**: linear model learned in embedding space. **Bottom left**: decision surface of the same model in input (linear) space.

A **self-explainable neural network** has the form:

$$p_\theta(1 \mid \mathbf{x}) = \sigma\Big(\underbrace{\sum_i w_i(\mathbf{x})\phi_i(\mathbf{x})}_{\text{"score" of } \mathbf{x}} \Big)$$

where:

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- Linear models associated to nearby inputs $\mathbf{x}$ **encouraged to be similar**, i.e., in the neighborhood of any $\mathbf{x}_0$ there exists a constant vector $\mathbf{w}_0$ that depends only on $\mathbf{x}_0$ and a “large enough” $\alpha > 0$ such that:

$$\sum_i w_i(\mathbf{x}')\phi_i(\mathbf{x}') \approx \sum_i w_{0i}\phi_i(\mathbf{x}_0) \qquad \text{for all } \mathbf{x}' \text{ that are closer than } \alpha \text{ to } \mathbf{x}_0$$

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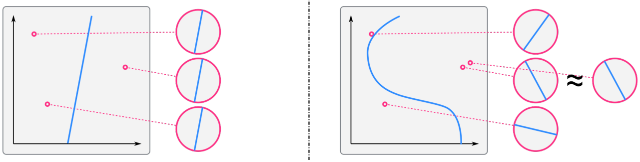
- If $\mathbf{w}(\mathbf{x}) \equiv \mathbf{w}$ is **constant** w.r.t. $\mathbf{x}$, we obtain a linear model again

- **Left**: a linear model. Notice that the weights $\mathbf{w}$ are constant everywhere.

- **Right**: a SENN. Notice that **locally** the weights $\mathbf{w}(\mathbf{x})$ are almost identical!



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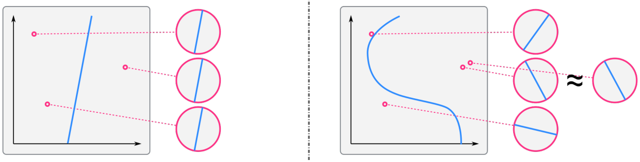


- SENNs are stable locally (**interpretability**) but flexible globally (**large capacity**)

- How to ensure that $\mathbf{w}(\mathbf{x})$ is "locally linear"?

Taylor's approximation for vector-valued functions

Let $\mathbf{w}(\mathbf{x})$ be a vector-valued function of a vector input $\mathbf{x}$. Taylor's theorem implies that $\mathbf{w}$ can be approximated around any $\mathbf{x}_0$ as:

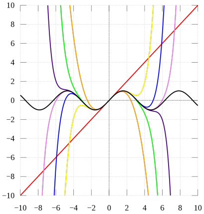
$$\mathbf{w}(\mathbf{x}) = \mathbf{w}(\mathbf{x}_0) + \underbrace{J(\mathbf{x}-\mathbf{x}_0)}_{\text{first-order term}} + \underbrace{\cdots}_{\text{quadratic+ terms}}$$

where J is the **matrix** of derivatives $J_{ab} = \frac{\partial w_a}{\partial x_b}$.

- The approximation is actually **exact for linear functions**:

$$\mathbf{w}^\top \mathbf{x} = \mathbf{w}^\top \mathbf{x}_0 + J(\mathbf{x}-\mathbf{x}_0)$$

- If we want $\mathbf{w}(\mathbf{x})$ to behave like a linear function we should minimize the contribution of the **quadratic term**, but doing so directly is challenging.



Taylor decomposition of a one-dimensional function, namely $\sin x$. The original function can be viewed as a (weighted) sum of the 1st, 2nd, 3rd, etc. **derivatives** of the function.

Credits: Wikimedia.

Idea: *regularize the model to approximate its own first-order Taylor expansion*

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A SENN with **parameters** θ (including the params of $\mathbf{w}(\mathbf{x})$ and of $\phi(\mathbf{x})$) is trained by minimizing:

$$\frac{1}{|S|} \sum_{(\mathbf{x},y) \in S} - \log p_\theta(y \mid \mathbf{x}) + \lambda \cdot \Omega(\theta, \mathbf{x})$$

where the **regularizer** Ω penalizes $\mathbf{w}(\mathbf{x})$ for **local deviations from linearity**:

$$\Omega(\theta, \mathbf{x}) := \| \underbrace{\nabla_\mathbf{x} p_\theta(1 \mid \mathbf{x})}_{\text{neural net analogue of weights}} - \underbrace{J\, \phi_\theta(\mathbf{x})}_{\text{if } f \text{ were linear}} \|$$

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■ Conceptually similar to tree-regularization, but with **linear models** in place of DTs. It is actually much faster because the regularizer does **not** require to learn DTs during training & Jacobian can be computed relatively quickly using autodiff packages.

Learning the Embedding Function $\phi(\mathbf{x})$

Idea: *learn to map* $\mathbf{x}$ *to* **interpretable** *concepts* ϕ. Strict requirement! Recall that an explanation looks like:

$$\big(w_1(\mathbf{x}) : \phi_1(\mathbf{x}), \quad \ldots, w_d(\mathbf{x}) : \phi_n(\mathbf{x})\big)$$

If $\phi_i(\mathbf{x})$ has clear semantics (e.g., "document $\mathbf{x}$ is about `politics`") this is a valid explanation, otherwise (e.g., for BERT embeddings) it is not!

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A minimal set of **desiderata**:

1. **Fidelity**: the representation of $\mathbf{x}$ in terms of concepts should **preserve relevant information**
2. **Diversity**: inputs should be representable with **few**, **non-overlapping** concepts
3. **Grounding**: concepts should have an immediate **human-understandable** interpretation.

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Remark: **nobody** knows how to formalize/implement the last desideratum properly!

- There are a few alternatives. One is to assume that $\phi(\cdot)$ is defined **manually by a domain expert**:

Example

Consider a medical diagnosis setting. A medical doctor could tell you that `lorazepam` is an important feature for predicting `clinical depression`. This can be modelled as a feature of the form:

$$\phi_3(\mathbf{x}) = \mathbb{1}(\text{the clinical record } \mathbf{x} \text{ reports administration of } \texttt{lorazepam})$$

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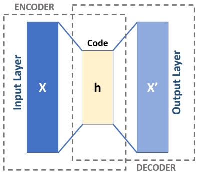
- Or, ideally, learn $\phi(\cdot)$ **jointly with the rest of the model**. How?

- Model $\phi(\cdot)$ using an **autoencoder**:



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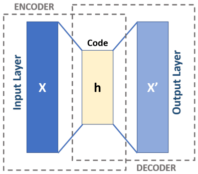

An **autoencoder** is defined as an encoder-decoder pair (ϕ, ψ):

$$\phi : \mathbb{R}^d \to \mathbb{R}^k \qquad \psi : \mathbb{R}^k \to \mathbb{R}^d$$

Encoder and decoder are trained jointly to minimize *reconstruction loss* $\ell_{\text{rec}}(\mathbf{x}, \mathbf{x}') = \sum_{j \in [d]} (x_i - x_i')^2$

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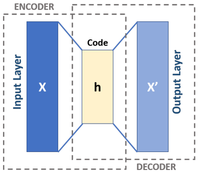

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$$\frac{1}{|S|} \sum_{(\mathbf{x},y) \in S} \{-p_\theta(y \mid \mathbf{x}) + \lambda \cdot \Omega(\theta, \mathbf{x}) + \lambda' \cdot \ell_{\text{rec}}(\mathbf{x}, \psi(\phi(\mathbf{x})))\}$$

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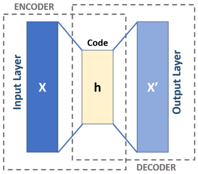

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- This encourages ϕ to satisfy **fidelity**, i.e., preserving both task-relevant information (because of the cross-entropy loss) and instance-relevant information (because of ℓ_{rec})

The complete architecture of a SENN is:

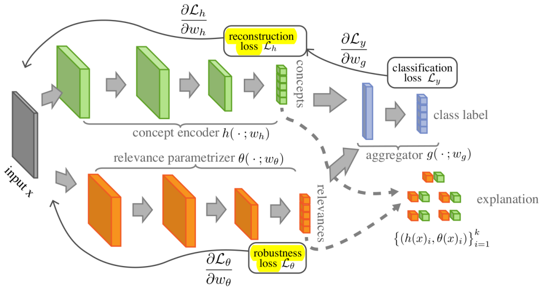

Figure 1: A SENN consists of three components: a **concept encoder** (green) that transforms the input into a small set of interpretable basis features; an **input-dependent parametrizer** (orange) that generates relevance scores; and an **aggregation function** that combines to produce a prediction. The robustness loss on the parametrizer encourages the full model to behave locally as a linear function on $h(x)$ with parameters $\theta(x)$, yielding immediate interpretation of both concepts and relevances.

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    * **synthetic prototypes**, i.e., inputs $\mathbf{x}$ that maximally activate one concept without activating the others:

    $$\mathbf{x}^{(j)} = \operatorname*{argmax}_{\mathbf{x}\in\mathbb{R}^d}\ \phi_j(\mathbf{x}) - \sum_{k\neq j}\phi_j(\mathbf{x})$$

    In practice, approximated using gradient ascent or similar techniques.

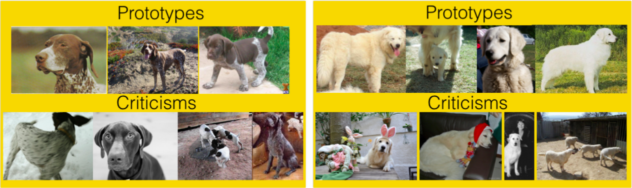
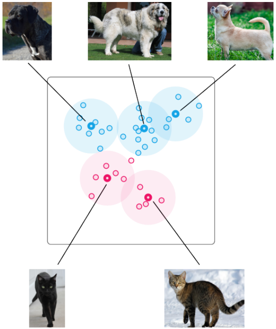


Figure 2: Learned prototypes and criticisms from Imagenet dataset (two types of dog breeds)

Is there a more **direct** way of incorporating prototypes and representation learning in an interpretable manner?

Prototypes + Deep Learning

- A **prototype** is an example that is prototypical of a certain class.



- **Example**: in a dog vs. cat image classification problem, the prototypes for the dog class correspond to prototypical images of dogs (e.g., a chihuahua, a mastiffs, . . .) that have "average features".

- Formally, a prototype is an example that is **close** (or **similar**) to many examples of the corresponding class, s.t. taken together they manage to "cover" all examples of that class. Distance is computed in, e.g., embedding space.

They can be found by clustering the data of a given class, for instance using k-means or other clustering algorithms.

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- Fix a distance function $d(\phi, \phi')$, compute **vector of distances** from class centroids:

$$\mathbf{d} = (d(\phi(\mathbf{x}), \mathbf{c}^1), \dots, d(\phi(\mathbf{x}), \mathbf{c}^v))$$

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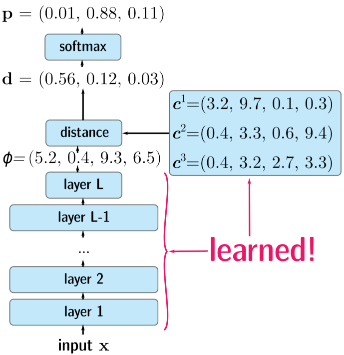
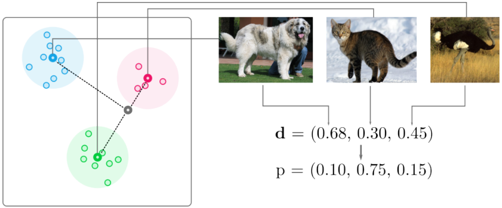
- Predicted **probability** of $\mathbf{x}$ belonging to class y proportional to **distance from prototype of that class**:

$$p_\theta(y \mid \mathbf{x}) := \mathrm{softmax}(-\mathbf{d})_y = \frac{\exp(-d(\phi(\mathbf{x}), c^y))}{\sum_{y'} \exp(-d(\phi(\mathbf{x}), c^{y'}))}$$

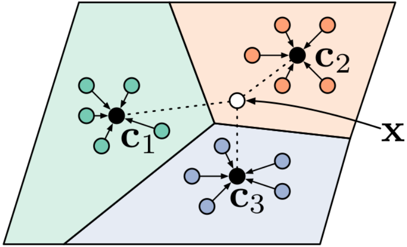
- Set of **all** parameters is $\theta = \{\phi, \mathbf{c}^1, \ldots, \mathbf{c}^v\}$.



- *Very* simple architecture



- And also *very* explainable! The probability of each class can be traced back to the corresponding prototype!



- During training both the **space** in which the embeddings live (determined by the lower layer) *and* the prototypes $\mathbf{c}^k$ are learned jointly!

- Fit ϕ by minimizing cross-entropy on the training set:

$$\text{argmin}_{\phi,\{\mathbf{c}^1,\ldots,\mathbf{c}^V\}} \; -\frac{1}{|S|}\sum_{(\mathbf{x},y)\in S} \log p_\theta(y \mid \mathbf{x})$$

[2] See: https://en.wikipedia.org/wiki/LogSumExp

- Fit ϕ by minimizing cross-entropy on the training set:

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The negative log-likelihood at a training example $(\mathbf{x}, y)$ is:

$$
\begin{aligned}
-\log p_\theta(y \mid \mathbf{x}) &= -\log \mathrm{softmax}(-\mathbf{d})_y && (1)\\
&= -\log \frac{\exp(-d(\phi(\mathbf{x}), \mathbf{c}^y))}{\sum_{y'} \exp(-d(\phi(\mathbf{x}), \mathbf{c}^{y'}))} && (2)\\
&= -\{\log \exp(-d(\phi(\mathbf{x}), \mathbf{c}^y)) - \log \sum_{y'} \exp(-d(\phi(\mathbf{x}), \mathbf{c}^{y'}))\} && (3)\\
&= -\{-d(\phi(\mathbf{x}), \mathbf{c}^y) - \log \sum_{y'} \exp(-d(\phi(\mathbf{x}), \mathbf{c}^{y'}))\} && (4)\\
&= d(\phi(\mathbf{x}), \mathbf{c}^y) + \log \sum_{y'} \exp(-d(\phi(\mathbf{x}), \mathbf{c}^{y'})) && (5)
\end{aligned}
$$

[2] See: https://en.wikipedia.org/wiki/LogSumExp

- Fit ϕ by minimizing cross-entropy on the training set:

$$\text{argmin}_{\phi, \{\mathbf{c}^1, \ldots, \mathbf{c}^v\}} \; -\frac{1}{|S|} \sum_{(\mathbf{x},y)\in S} \log p_\theta(y \mid \mathbf{x})$$

The negative log-likelihood at a training example $(\mathbf{x}, y)$ is:

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The first element is the distance to the prototype of class y. The second element is the “soft maximum” of the negative distances to other classes [2]:

$$\max\{-d_1, \ldots, -d_v\} \leq \log \sum_{y'} \exp(-d_{y'}) \leq \max\{-d_1, \ldots, -d_v\} + \log(v)$$

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Minimizing this implies (i) min. distance to true class y and (ii) approx. max. distance to other classes.

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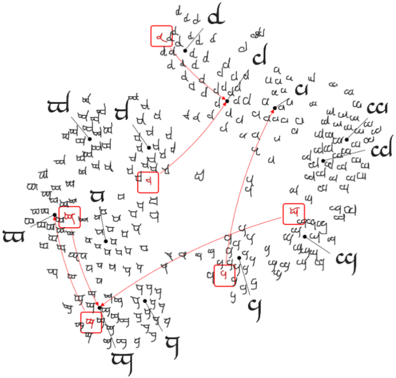

Figure 2: A t-SNE visualization of the embeddings learned by Prototypical networks on the Omniglot dataset. A subset of the Tengwar script is shown (an alphabet in the test set). Class prototypes are indicated in black. Several misclassified characters are highlighted in red along with arrows pointing to the correct prototype.

- *Very* clear results

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+/- Designed for **few-shot regime**
  - Only *one* prototype per class
  - Works well if few examples, poorly if many

Architecture of **prototype classification networks** (PCNs)

- **Autoencoder**:

  Encoder: $f : \mathbb{R}^p \to \mathbb{R}^q, \mathbf{z} := f(\mathbf{x})$ Decoder: $g : \mathbb{R}^q \to \mathbb{R}^p, \hat{\mathbf{x}} := g(\mathbf{z})$

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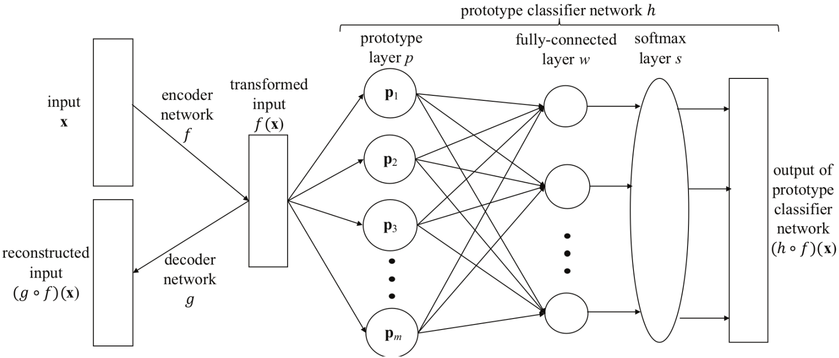
- **Dense Layer** + **Softmax**

$$p_\theta(y \mid \mathbf{x}) = \mathrm{softmax}(Wp(f(\mathbf{x})))_y = \frac{\exp \mathbf{w}^{(y)} \cdot \mathbf{p}(f(\mathbf{x}))}{\exp \sum_{y'} \mathbf{w}^{(y')} \cdot \mathbf{p}(f(\mathbf{x}))}$$

Prototype Classification Networks



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- PCNs recover ProtoNets if one prototype per class and W is *fixed* to $-I$

- The PCN loss is a **weighted sum** of several terms:
    - Classification loss, like the negative log-likelihood:

$$-\frac{1}{|S|}\sum_{(\mathbf{x},y)\in S} \log p_\theta(y \mid \mathbf{x}) = -\frac{1}{|S|}\sum_{(\mathbf{x},y)\in S}\sum_k \mathbb{1}(y=k)\log p_\theta(k \mid \mathbf{x})$$

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- In practice min over S restricted to mini-batch.

Learned Prototypes

Figure 2: Some random images from the training set in the first row and their corresponding reconstructions in the second row.

Figure 3: 15 learned MNIST prototypes visualized in pixel space.

Figure 9: 15 decoded prototypes for Fashion-MNIST.

Learned Prototypes

	interpretable	non-interpretable
train acc	98.2%	99.8%
test acc	93.5%	94.2%

Table 3: Car dataset accuracy.

Figure 5: Decoded prototypes when we include R_1 and R_2.

- Cars dataset – contains small B/W images of cars from different angles.
- **High performance** without entirely sacrificing interpretability.

	0	1	2	3	4	5	6	7	8	9
	-0.07	7.77	1.81	0.66	4.01	2.08	3.11	4.10	-20.45	-2.34
	2.84	3.29	1.16	1.80	-1.05	4.36	4.40	-0.71	0.97	-18.10
	-25.66	4.32	-0.23	6.16	1.60	0.94	1.82	1.56	3.98	-1.77
	-1.22	1.64	3.64	4.04	0.82	0.16	2.44	-22.36	4.04	1.78
	2.72	-0.27	-0.49	-12.00	2.25	-3.14	2.49	3.96	5.72	-1.62
	-5.52	1.42	2.36	1.48	0.16	0.43	-11.12	2.41	1.43	1.25
	4.77	2.02	2.21	-13.64	3.52	-1.32	3.01	0.18	-0.56	-1.49
	0.52	-24.16	2.15	2.63	-0.09	2.25	0.71	0.59	3.06	2.00
	0.56	-1.28	1.83	-0.53	-0.98	-0.97	-10.56	4.27	1.35	4.04
	-0.18	1.68	0.88	2.60	-0.11	-3.29	-11.20	2.76	0.52	0.75
	5.98	0.64	4.77	-1.43	3.13	-17.53	1.17	1.08	-2.27	0.78
	1.53	-5.63	-8.78	0.10	1.56	3.08	0.43	-0.36	1.69	3.49
	1.71	1.49	-13.31	-0.69	-0.38	4.55	1.72	1.59	3.18	2.19
	5.06	-0.03	0.96	4.35	-21.75	4.25	1.42	-1.27	1.64	0.78
	-1.31	-0.62	-2.69	0.96	2.36	2.83	2.76	-4.82	-4.14	4.95

Table 1: Transposed weight matrix (every entry rounded off to 2 decimal places) between the prototype layer and the softmax layer. Each row represents a prototype node whose decoded image is shown in the first column. Each column represents a digit class. The most negative weight is shaded for each prototype. In general, for each prototype, its most negative weight is towards its visual class except for the prototype in the last row.

- Interpretation of prototype-class weights for MNIST

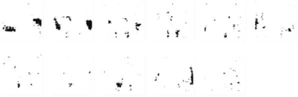

Figure 6: Decoded prototypes when we remove R_1 and R_2.

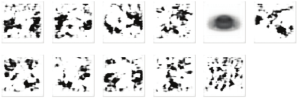

Figure 7: Decoded prototypes when we remove R_1.

- Disabling the regularizers **hinders** interpretability of the prototypes

- Is autoencoding the way to go?

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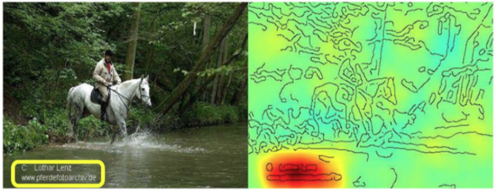
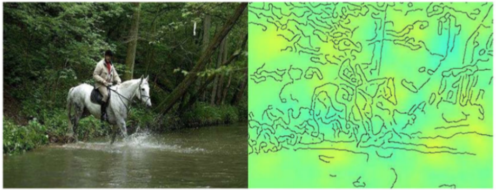
- Can we go beyond concrete prototypes and look at *where* certain prototypes activate?

Horse-picture from Pascal VOC data set



Source tag present → Classified as horse



No source tag present → Not classified as horse

■ How would you describe why the image looks like a “clay colored sparrow”?

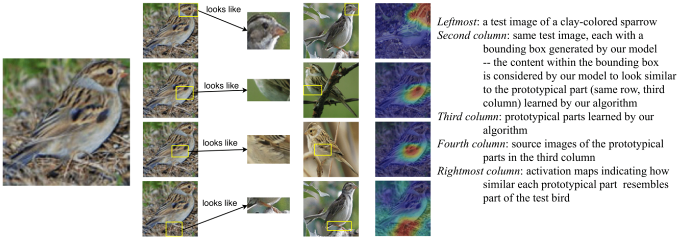


Figure 1: Image of a clay colored sparrow and how parts of it look like some learned prototypical parts of a clay colored sparrow used to classify the bird’s species.

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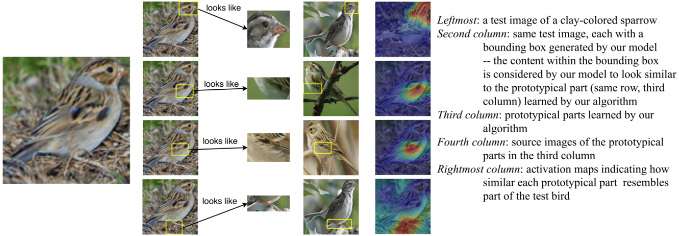

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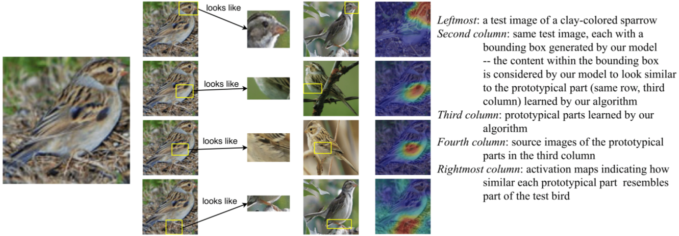

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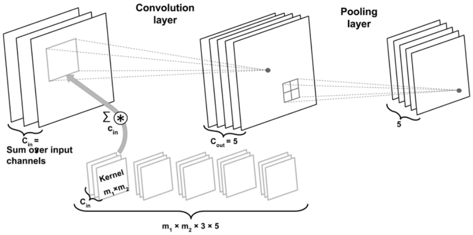
Idea: enable models to focus on parts of the image and compare them with prototypical parts of training images from a class – reasoning of the form “this looks like that”



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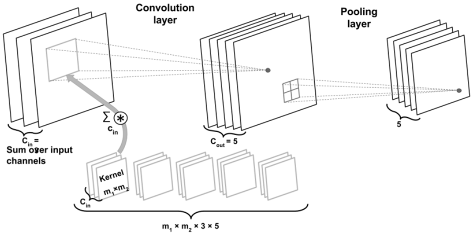
  - Given an **input** x of size $w \times h \times c$



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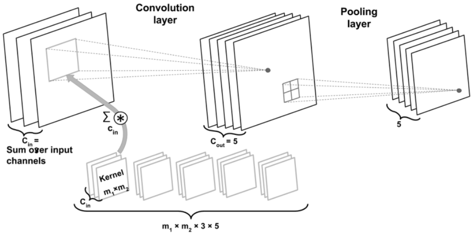

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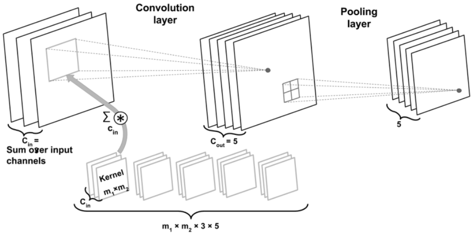

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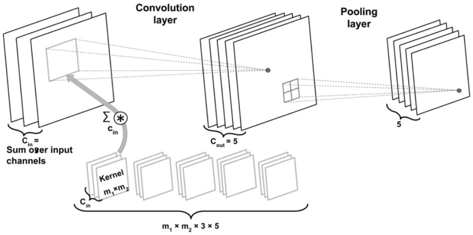
  - The outputs $y_1, \ldots, y_d$ are **stacked** to obtain the complete $a \times b \times d$ embedding y
- The size of the kernel is the **receptive field** of the convolutional layer

Refresher: Convolutional Networks



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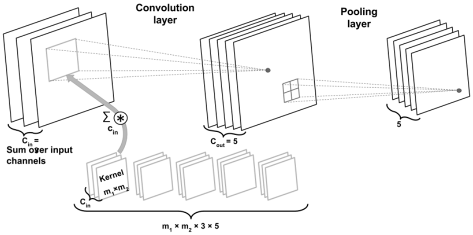

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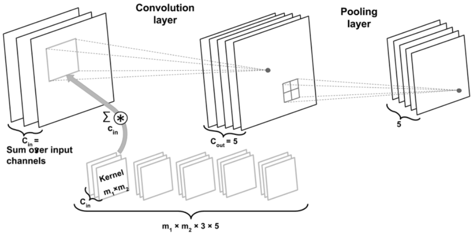

- Convolutional filters take an input, typically reduce its size, and output a variable number of channels (depth)
- Pooling layers behave similarly but aggregate their inputs using max or avg, and have no learnable parameters
- CNNs stack convolutional layers intermixed with pooling layers (e.g., max activations) on top of each other to produce a latent representation:

$$w \times h \times c \quad \longrightarrow \quad w' \times h' \times d$$

- Consider convolutional embeddings $\mathbf{z} = f(\mathbf{x})$:

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- In ProtoNets and PCNs, a **prototype** $\mathbf{p} \in \mathbb{R}^{w' \times h' \times d}$ is a point in embedding space:
  - Summarizes a **set** of **examples**
  - Distance from **prototype** used as activation
  - Interpretability achieved by ensuring that $\mathbf{p}$ is "close" to **concrete example**

- Consider convolutional embeddings $\mathbf{z} = f(\mathbf{x})$:

$$w \times h \times c \quad \longrightarrow \quad w' \times h' \times d$$

with $w' \leq w$ and $h' \leq h$

- In ProtoNets and PCNs, a **prototype** $\mathbf{p} \in \mathbb{R}^{w' \times h' \times d}$ is a point in embedding space:
  - Summarizes a **set** of **examples**
  - Distance from **prototype** used as activation
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- In PPNets, a **part-prototype** $\mathbf{p} \in \mathbb{R}^{1 \times 1 \times d}$ is a *part* of a point in embedding space
  - Summarizes a **set** of **example parts**
  - Distance from **part-prototype** used as activation
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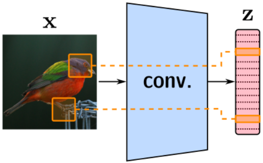
ProtoPNets (Chen et al., 2019)

- **ProtoPNets** are a class of "gray-box" models that aim at achieveing high-performance through **representation learning** while providing **faithful** explanations for their own predictions.



- Embed input image $\mathbf{x}$ using convolutional layers → each "tube" in the latent representation can be mapped back to a region of the image.

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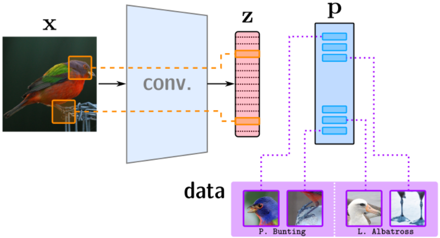

- Jointly learn *k* **part-prototypes** for each class, i.e., "tubes" of latent representations of **parts of concrete training examples**. Learned using typical clustering losses (coverage & separation).

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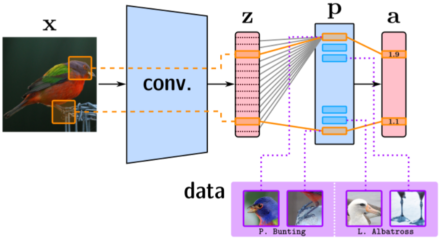

- During inference, input "tubes" are compared to learned part-prototypes (also "tubes") and their similarity is computed - this captures similarity information between the input and training examples.

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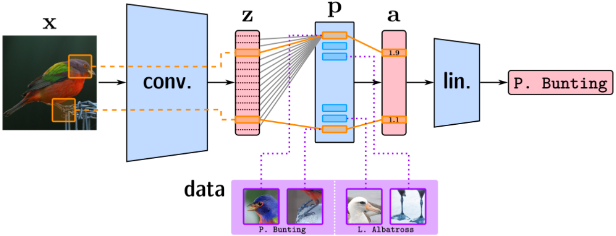

- The similarities themselves are passed through a linear layer and a `softmax` activation to obtain a distribution over classes.

Architecture of **part-prototype networks** (PPNets)

- **Embedding** function [**it was an autoencoder**]

$$f : \mathbb{R}^{w \times h \times c} \rightarrow \mathbb{R}^{w' \times h' \times d}$$

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- **Dense Layer** + **Softmax** [**same**]

$$p_\theta(y \mid \mathbf{x}) = \mathrm{softmax}(W\mathbf{a}(f(\mathbf{x})))_y = \frac{\exp \mathbf{w}^{(y)} \cdot \mathbf{a}^{(y)}(f(\mathbf{x}))}{\exp \sum_{y'} \mathbf{w}^{(y')} \cdot \mathbf{a}^{(y')}(f(\mathbf{x}))}$$

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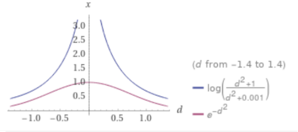
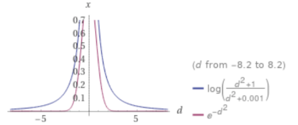
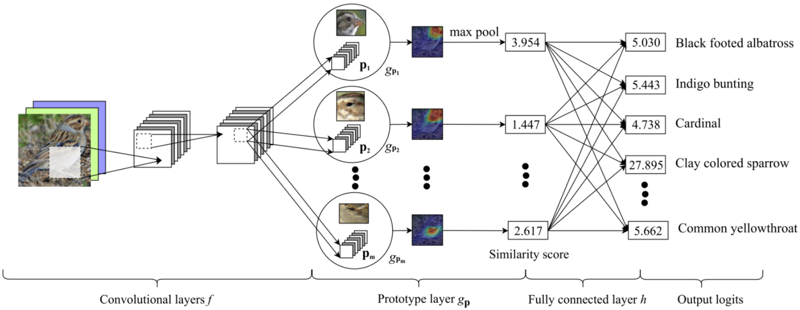




Comparison between difference-of-logs and Gaussian of d:

$$\text{act}'(\mathbf{p}, \widetilde{\mathbf{z}}) = \exp\left(-\gamma \cdot d(\mathbf{p}, \widetilde{\mathbf{z}})^2\right)$$

In the plot $\epsilon = 0.001$, $\gamma = 1$



Remark:

- Convolutional filters slide over the input (first step from the left)
- Part-prototypes slide over the embeddings (second step from the left)

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$$\Omega_{cls} := \frac{1}{|S|} \sum_{(\mathbf{x},y)\in S} \min_{\mathbf{p}\in\mathrm{pps}_y} \min_{\widetilde{\mathbf{z}}\in\mathrm{parts}(f(\mathbf{x}))} \|\mathbf{p} - \widetilde{\mathbf{z}}\|^2$$

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$$\mathbf{p}_{\text{new}} \leftarrow \operatorname*{argmin}_{\mathbf{p}_{\text{new}} \in \mathcal{Q}^{(y)}} \|\mathbf{p}_{\text{new}} - \mathbf{p}\|^2$$

where:

$$\mathcal{Q}^{(y)} = \{\widetilde{\mathbf{z}} \ : \ \widetilde{\mathbf{z}} \in \mathrm{parts}(f(\mathbf{x}_i)), \ y_i = y\}$$

is the set of all parts of (latent representations of) instances $\mathbf{x}_i$ in the prototype's class.

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- Solved using SGD or similar.

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    At this stage, fix the weight vectors of the top dense layer to:

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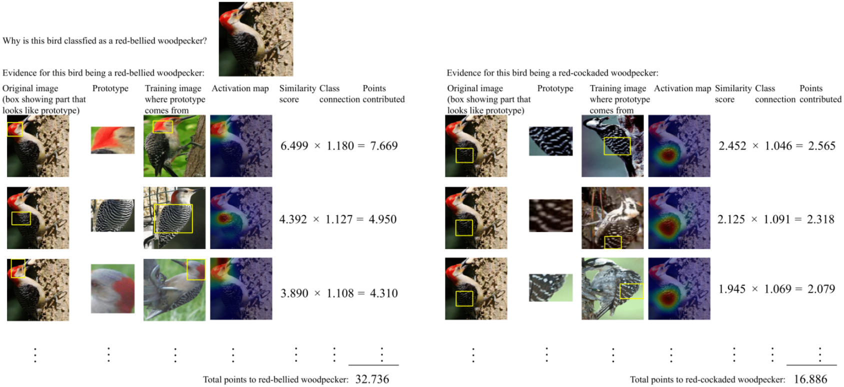
  - Periodically push prototypes close to training examples.
  - Once f and $\{\mathbf{p}\}$ are found, optimize weights of top dense layer W by optimizing the cross-entropy loss $\rightarrow$ convex problem

Example



- Not quite counterfactual, but useful

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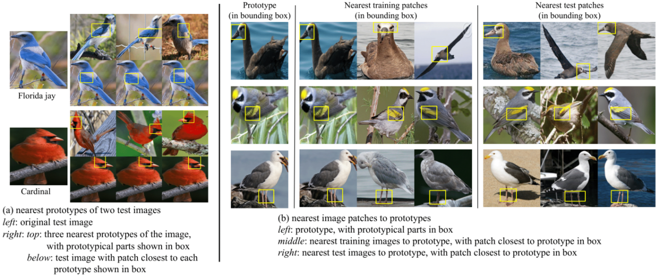

Figure 5: Nearest prototypes to images and nearest images to prototypes. The prototypes are learned from the training set.

- PPNets are the only method that explains where prototypes activate *and* where they come from!

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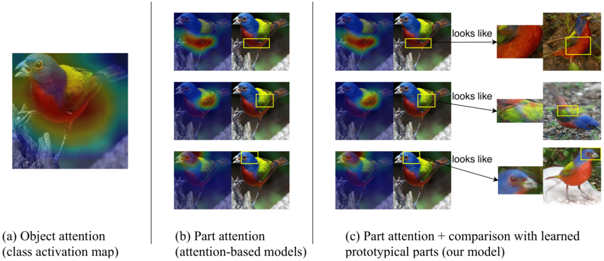

Figure 4: Visual comparison of different types of model interpretability: (a) object-level attention map (e.g., class activation map [56]); (b) part attention (provided by attention-based interpretable models); and (c) part attention with similar prototypical parts (provided by our model).

- Comparison between PPNets and other approaches to explainability

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- The concepts $\{c_j\}$ are:
  - Learned from data so to be discriminative and interpretable.
  - Black-box: what's "above" the concepts is interpretable, what's "underneath" is not.

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Remarks:

- The concepts and the weights are both integral to the explanation:
  - Concepts $\{c_j\}$ establish a vocabulary that enables communication with stakeholders
  - Weights $\{w_j(\mathbf{x})\}$ convey the relative importance of different concepts
- The prediction $y = f(\mathbf{x})$ is independent from $\mathbf{x}$ given the explanation $\text{expl}(\mathbf{x}, y) \rightarrow$ the explanations is 100% **faithful** to the model's decision process.

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- Am I Dreaming? *Kinda :-(*
- *Interpretability not well defined!*
- Each CBM implements it in its own way:
  - Activation sparsity
  - Orthonormality
  - Similarity to concrete examples
  - ... all *unsupervised* approaches

Concept Bottleneck Models

Pang Wei Koh [*1] **Thao Nguyen** [*1 2] **Yew Siang Tang** [*1]
Stephen Mussmann [1] **Emma Pierson** [1] **Been Kim** [2] **Percy Liang** [1]

Abstract

We seek to learn models that we can interact with using high-level concepts: if the model did not think there was a bone spur in the x-ray, would it still predict severe arthritis? State-of-the-art models today do not typically support the manipulation of concepts like “the existence of bone spurs”, as they are trained end-to-end to go directly from raw input (e.g., pixels) to output (e.g., arthritis severity). We revisit the classic idea of first predicting concepts that are provided at training time, and then using these concepts to predict the label. By construction, we can intervene on these *concept bottleneck models* by editing their predicted concept values and propagating these changes to the final prediction. On x-ray grading and bird identification, concept bottleneck models achieve competitive accuracy with standard end-to-end models, while enabling interpretation in terms of high-level clinical concepts (“bone spurs”) or bird attributes (“wing color”). These

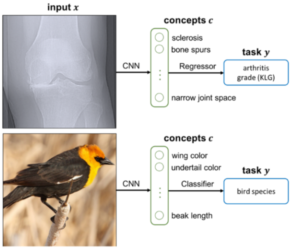

Figure 1. We study concept bottleneck models that first predict an intermediate set of human-specified concepts c, then use c to predict the final output y. We illustrate the two applications we consider: knee x-ray grading and bird identification.

(Source: (Koh et al., 2020) Also: Concept Whitening (Chen et al., 2020))

Concept Annotations Are Not Enough!

DO CONCEPT BOTTLENECK MODELS LEARN AS INTENDED?

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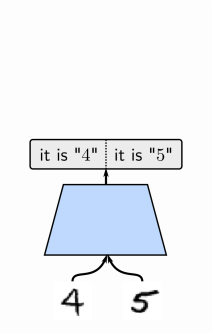
ABSTRACT

Concept bottleneck models map from raw inputs to concepts, and then from concepts to targets. Such models aim to incorporate pre-specified, high-level concepts into the learning procedure, and have been motivated to meet three desiderata: interpretability, predictability, and intervenability. However, we find that concept bottleneck models struggle to meet these goals. Using post hoc interpretability methods, we demonstrate that concepts do not correspond to anything semantically meaningful in input space, thus calling into question the usefulness of concept bottleneck models in their current form.

(Source: (**??**))

Concept Leakage = Unintended Semantics

① Fit two concepts to recognize `MNIST` images of "4"s and "5"s using **full concept annotations**



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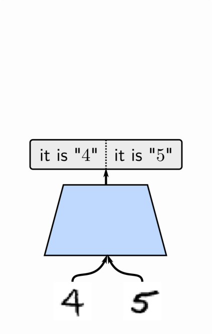
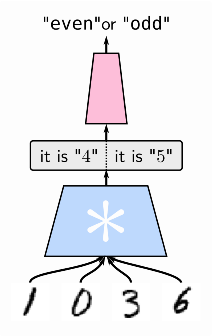


② Use the learned concepts, predict parity of **remaining digits** (i.e., all except "4" and "5")



- Performance is **much better than random**!

Take-away

- Concept-based models combine features of white and black-box models:
  - **Interpretability** (for parts of the prediction process)
  - **Faithfulness** of the produced explanations, they come for **free**
  - **High performance** on non-tabular data, thanks to representation learning
- **SENNs** upgrade linear models to representation learning; not 100% clear how to learn **interpretable concepts**
- Prototype and part-prototype models (partially) solve this issue by **mapping prototypes to examples** (or **parts of examples**)
- Still very much an **open area of research**! (Especially ensuring that concepts are interpretable)

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