Gray-box Models

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Advanced Machine Learning Course

White-box models:

- + Many well-known examples (e.g., shallow DTs, sparse linear models, rules lists)
- + Make explanations available for free
- + Applicable to tabular data only
- - Generally no support for representation learning
- - Low performance on non-tabular data

Black-box models:

+ Many well-known examples (e.g., neural nets, ensemble methods, non-linear kernel methods)
+ High performance on non-tabular data like images and text
+ Support for advanced representation learning
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- Gradient-based expl. are point-wise can be contradictory or ambiguous
- Perturbation-based expl. are expensive to compute and can have high variance
+ Do not require modifying/retraining the model $\leftarrow$ *is this always necessary?*

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 go **generalize** this strategy?

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$$p_\theta(y \mid \mathbf{x}) := (\mathrm{extract}_y \circ \mathrm{softmax} \circ \mathbf{w}^{(y)} \circ \boldsymbol{\phi})(\mathbf{x})$$

where $\phi(\mathbf{x})$ are embeddings and $W(\phi)$ is a dense layer. Let $\ell(\theta, (\mathbf{x}, y))$ be a loss.

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Tree Regularization: minimize the regularized loss:

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

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- How to compute Ω? How to make optimize it?

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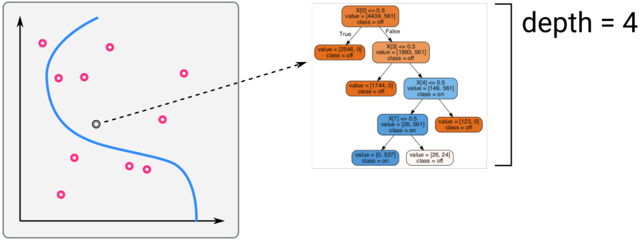
- Makes sense as long as $|Q| \ll |S|$
- Under the assumption that θ doesn't change "too much" across epochs, one can warm start training μ from the previous epoch.

An illustration:



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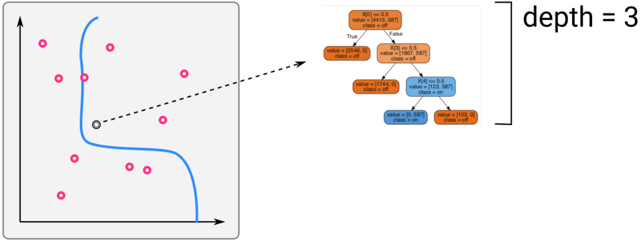

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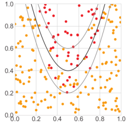
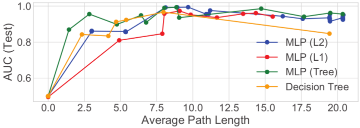
Example: Fitting a Parabola



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



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

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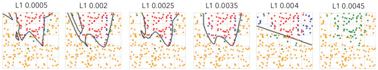
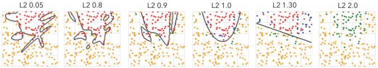
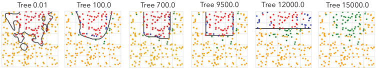
- For $\lambda = 9500$ (the exact value is not important) the tree-regularized network recovers exactly the shape of a **DT with depth** 2. Increasing λ further further flattens the tree to depth 1, at the cost of accuracy.



(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

Gray-box Model (GBM)

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
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We will see different classes of GBMs:

- Self-explainable Neural Networks (SENNs) [Alvarez-Melis and Jaakkola, 2018]
- Prototypical Nets (ProtoNets) [Snell et al., 2017]
- Prototype Classification Networks (PCNs) [Li et al., 2018]
- Part-Prototype Networks (PPNets) [Chen et al., 2019]

and discuss their **promise** and **issues**

Self-explainable Neural Networks

A **linear model** has the form:

$$f(\mathbf{x}) = \mathrm{sign}\big(\underbrace{\langle \mathbf{w}, \mathbf{x} \rangle + w_0}_{\text{"score" of } \mathbf{x}} \big), \qquad \langle \mathbf{w}, \mathbf{x} \rangle := \textstyle\sum_{i \in [d]} w_i x_i$$

A **sparse linear model** $\mathbf{w} \in \mathbb{R}^d$ contains few non-zero entries [Tibshirani, 1996, Ustun and Rudin, 2016]. 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:

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

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!

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- *What? Isn't this paradoxical?*

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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:

$$\langle \mathbf{w}(\mathbf{x}'), \boldsymbol{\phi}(\mathbf{x}') \rangle \approx \langle \mathbf{w}', \boldsymbol{\phi}(\mathbf{x}') \rangle \qquad \forall\ \mathbf{x}' \ .\ \|\mathbf{x}' - \mathbf{x}_0\| \leq \alpha$$

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where:

- $\phi : \mathbb{R}^d \to \mathbb{R}^k$ embeds inputs into feature space, **implemented as neural net!**
- $\mathbf{w} : \mathbb{R}^d \to \mathbb{R}^k$ computes a weight vector for each input, **implemented as neural net!**
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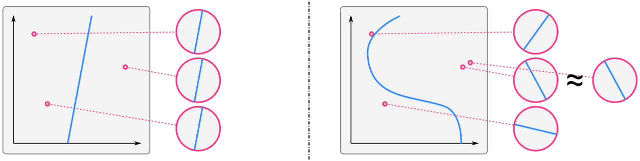

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Right: a SENN. The weight vector depends on $\mathbf{x}$ and nearby inputs have similar weight vectors.

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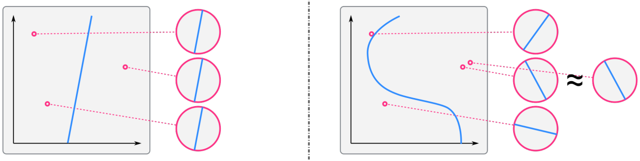

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Right: a SENN. The weight vector depends on $\mathbf{x}$ and nearby inputs have similar weight vectors.

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

In the **multi-class** case, SENNs take the form:

$$f(\mathbf{x}) = \operatorname*{argmax}_{y \in [v]} \ \mathrm{softmax}\left(\langle \mathbf{w}^{(y)}(\mathbf{x}), \boldsymbol{\phi}(\mathbf{x}) \rangle \right)$$

where the **neural net** $W(\mathbf{x}) = [\mathbf{w}^{(1)}(\mathbf{x}), \ldots, \mathbf{w}^{(v)}(\mathbf{x})]$ outputs a $c \times v$ matrix

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

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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:

$$\mathbf{w}(\mathbf{x}) = \mathbf{w}(\mathbf{x}_0) + J(\mathbf{x} - \mathbf{x}_0) + o(\|\mathbf{x} - \mathbf{x}_0\|)$$

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- If we want $\mathbf{w}(\mathbf{x})$ to behave like a linear function we should minimize the contribution of the **quadratic term**
- Directly minimizing the quadratic+ terms is **hard** (involves computing, e.g., Hessian)

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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:

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

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

$$\Omega(\theta, \mathbf{x}) := \| \underbrace{\nabla_{\mathbf{x}} \mathrm{score}(\mathbf{x})}_{\text{neural net analogue of weights}} - J\mathbf{w}(\mathbf{x}) \|$$

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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.

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Idea: *learn to map* x *to interpretable concepts* ϕ

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1. **Fidelity**: the representation of x in terms of concepts should **preserve relevant information**
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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:
  - Assume that $\phi(\cdot)$ is defined manually by a domain expert:
    Example: a medical doctor could tell you that `lorazepam` is an important feature for predicting `clinical depression`; makese sense for **tabular data**.

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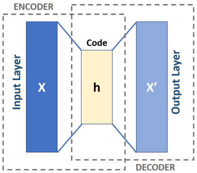
  - Learn $\phi(\cdot)$ **jointly** with the rest of the model. How?

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



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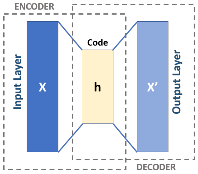

An **autoencoder** is defined as an encoder-decoder pair (ϕ, ψ):

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

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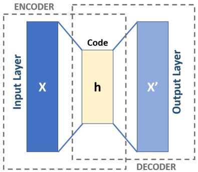

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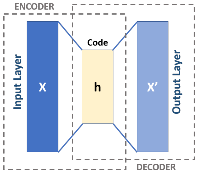

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- This encourages ϕ to satisfy **fidelity**, i.e., preserving both task-relevant information (because of ℓ) and instance-relevant information (because of ℓ_{rec})

The complete architecture of a SENN is:

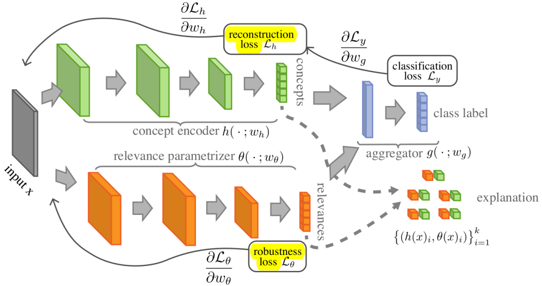

Figure 1: A SENN consists of three components: a **concept encoder** (green) that transforms the input into a small set of interpretable basis features; an **input-dependent parametrizer** (orange) that generates relevance scores; and an **aggregation function** that combines to produce a prediction. 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.

Recall that we minimize:

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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.

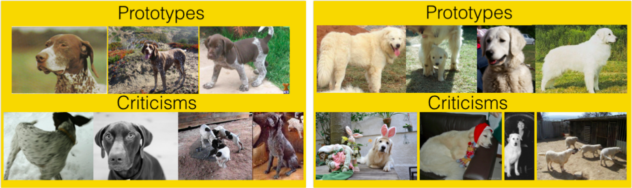

Figure 2: Learned prototypes and criticisms from Imagenet dataset (two types of dog breeds)

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

Prototypes + Deep Learning

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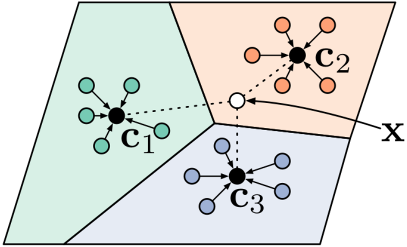
- Predicted **probability** of $\mathbf{x}$ belonging to class y defined as:

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

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



- *Very* simple architecture

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

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

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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]:

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

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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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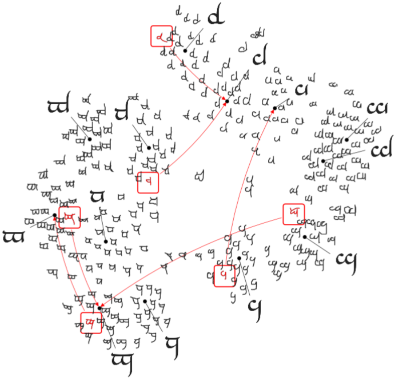

Figure 2: A t-SNE visualization of the embeddings learned by Prototypical networks on the Omniglot dataset. A subset of the Tengwar script is shown (an alphabet in the test set). Class prototypes are indicated in black. Several misclassified characters are highlighted in red along with arrows pointing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

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

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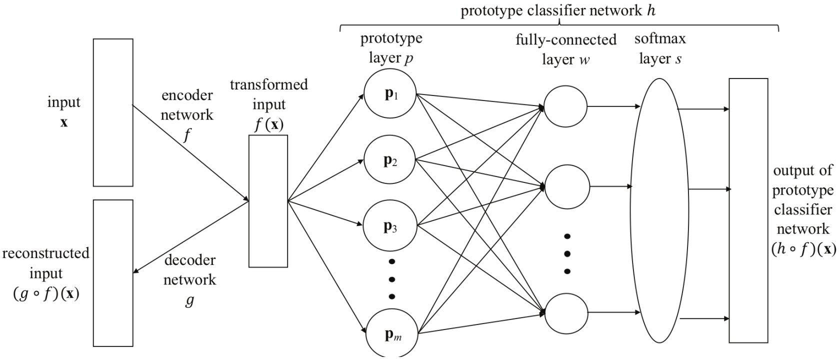
prototype classifier network h
input
$\mathbf{x}$
encoder
network
f
transformed
input
$f(\mathbf{x})$
reconstructed
input
$(g \circ f)(\mathbf{x})$
decoder
network
g
prototype
layer p
$\mathbf{p}_1$
$\mathbf{p}_2$
$\mathbf{p}_3$
$\mathbf{p}_m$
fully-connected
layer w
softmax
layer s
output of
prototype
classifier
network
$(h \circ f)(\mathbf{x})$

- ProtoNets:
  - Map $\mathbf{x}$ to space of emebeddings $\mathbb{R}^q$
  - Each class y is represented by **exactly one** centroid $\mathbf{c}^y \in \mathbb{R}^q$
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- PCNs are more **flexible**: possibly *multiple* prototypes per class
- 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.

Learned Prototypes

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

Effect of Regularizers

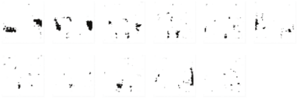

Figure 6: Decoded prototypes when we remove R_1 and R_2.

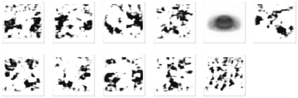

Figure 7: Decoded prototypes when we remove R_1.

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

- Is autoencoding the way to go?

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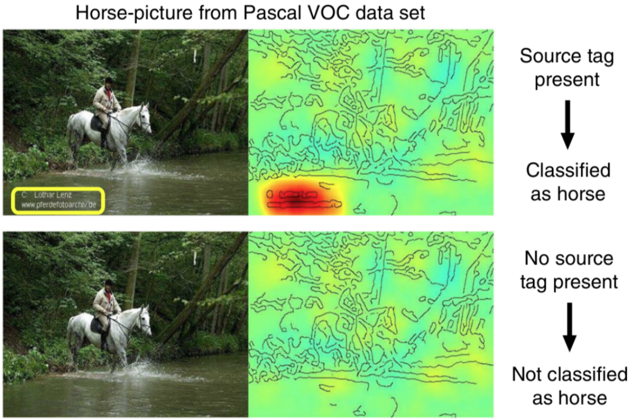
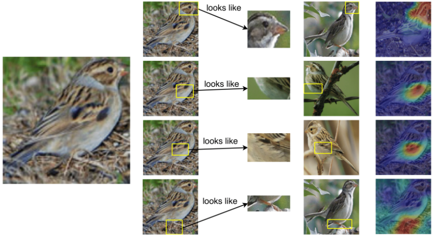
- Can we go beyond concrete prototypes and look at *where* certain prototypes activate?



- How would you describe why the image looks like a "clay colored sparrow"?



Leftmost: a test image of a clay-colored sparrow
Second column: same test image, each with a bounding box generated by our model -- the content within the bounding box is considered by our model to look similar to the prototypical part (same row, third column) learned by our algorithm
Third column: prototypical parts learned by our algorithm
Fourth column: source images of the prototypical parts in the third column
Rightmost column: activation maps indicating how similar each prototypical part resembles part of the test bird

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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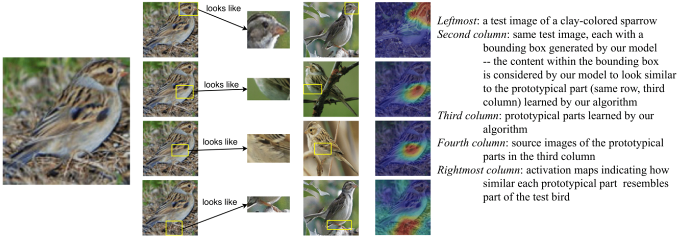

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- Perhaps bird’s **head** and **wing bars** *look like* those of a **prototypical** clay colored sparrow
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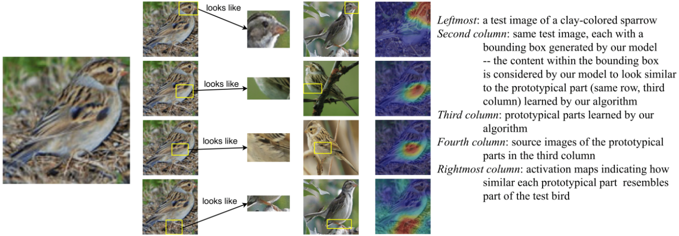

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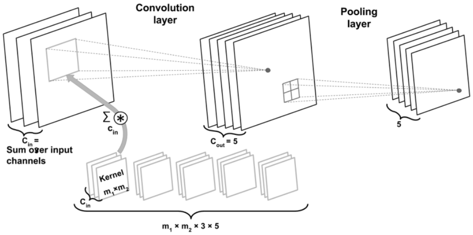
Idea: enable models to focus on parts of the image and compare them with prototypical parts of training images from a class – reasoning of the form "this looks like that"

Refresher: Convolutional Filters



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

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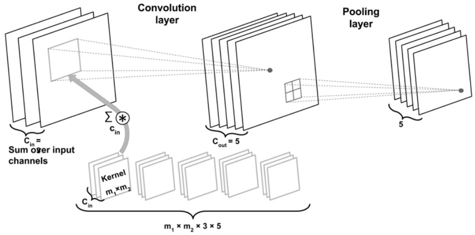

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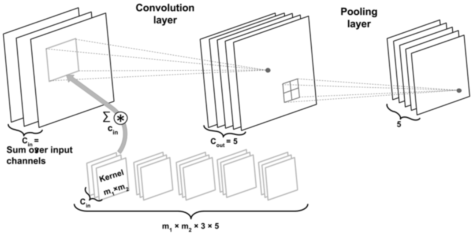

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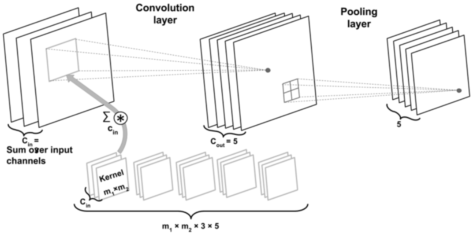

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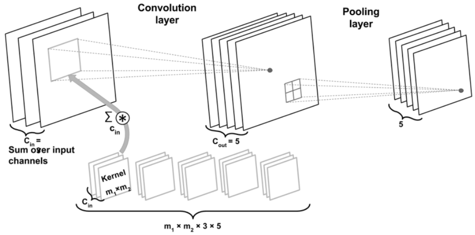
  - The outputs $y_1, \ldots, y_d$ are **stacked** to obtain the complete $a \times b \times d$ embedding y
- The size of the kernel is the **receptive field** of the convolutional layer



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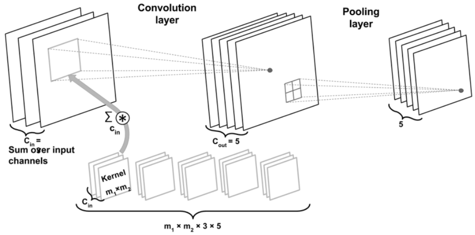

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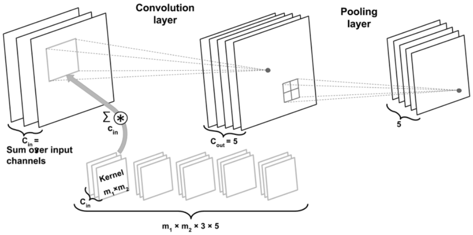

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- Pooling layers behave similarly but aggregate their inputs using max or avg, and have no learnable parameters
- CNNs stack convolutional layers intermixed with pooling layers (e.g., max activations) on top of each other to produce a latent representation:

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

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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
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  - Distance from **part-prototype** used as activation
  - Interpretability achieved by ensuring that $\mathbf{p}$ is "close" to concrete **example parts**

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

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

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

Loaded from a **pre-trained network**. Top layers can be **fine-tuned** while leaving the rest fixed (frozen).

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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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  - Define activation of $\mathbf{p}$ on full embeddings $\mathbf{z}$ as maximum activation of its parts:

  $$\mathrm{act}(\mathbf{p}, \mathbf{z}) = \max_{\widetilde{\mathbf{z}} \in \mathrm{parts}(\mathbf{z})} \mathrm{act}(\mathbf{p}, \widetilde{\mathbf{z}})$$

How to measure **activation** of **part**-prototype $\mathbf{p} \in \mathbb{R}^{1\times 1\times d}$ on a full embedding $\mathbf{z} \in \mathbb{R}^{w'\times h'\times d}$?

- Break down $\mathbf{z}$ into all its **pieces** $\widetilde{\mathbf{z}}$ of size $1 \times 1 \times d$, denoted:

$$\mathrm{parts}(\mathbf{z})$$

- Measure L_2 **distance** between $\mathbf{p}$ and each part $\widetilde{\mathbf{z}}$ of $\mathbf{z}$:

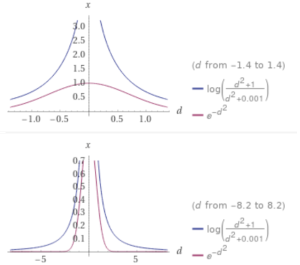
$$d(\mathbf{p}, \widetilde{\mathbf{z}}) = \|\mathbf{p} - \mathbf{z}\|$$

- Convert distance into **activation**:

$$\mathrm{act}(\mathbf{p}, \widetilde{\mathbf{z}}) = \log\left(\frac{d(\mathbf{p}, \widetilde{\mathbf{z}})^2 + 1}{d(\mathbf{p}, \widetilde{\mathbf{z}})^2 + \epsilon}\right)$$

- Define activation of $\mathbf{p}$ on full embeddings $\mathbf{z}$ as maximum activation of its parts:

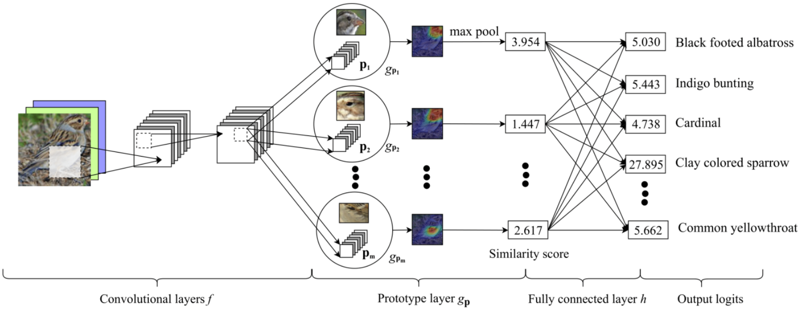
$$\mathrm{act}(\mathbf{p}, \mathbf{z}) = \max_{\widetilde{\mathbf{z}} \in \mathrm{parts}(\mathbf{z})} \mathrm{act}(\mathbf{p}, \widetilde{\mathbf{z}})$$



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

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

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)

- How to ensure that part-prototypes are class-specific?

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Desiderata:

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

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

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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$$\frac{1}{|S|} \sum_{(\mathbf{x},y) \in S} \ell_{\text{ce}}(\mathbf{x}, y) + \lambda_1 \Omega_{cls} + \lambda_2 \Omega sep$$

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

$$w_i^{(y)} = \begin{cases} 1 & \text{if } \mathbf{p}_i \text{ belongs to class } y \\ -\frac{1}{2} & \text{otherwise} \end{cases}$$

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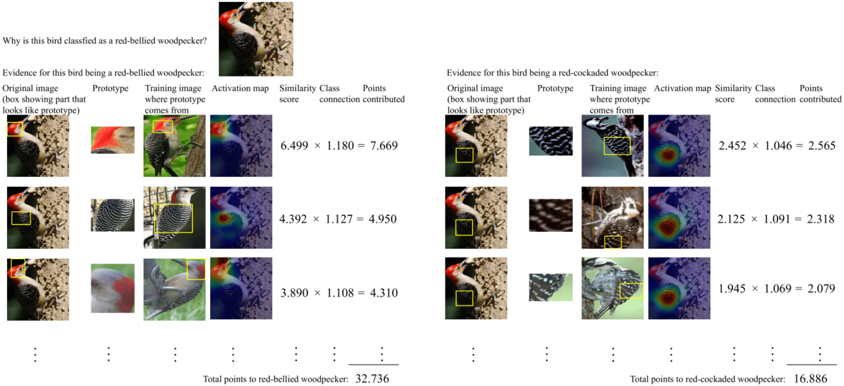
  - Once f and $\{\mathbf{p}\}$ are found, optimize weights of top dense layer W by optimizing the cross-entropy loss $\rightarrow$ convex problem

Example



- Not quite counterfactual, but useful

Example

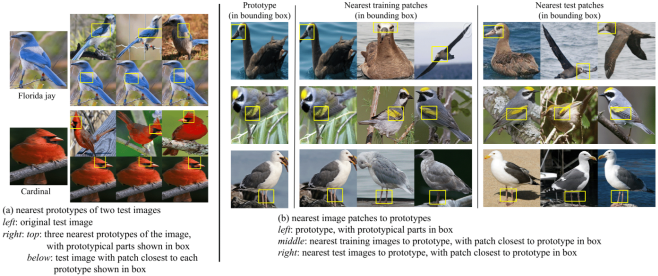


Figure 5: Nearest prototypes to images and nearest images to prototypes. The prototypes are learned from the training set.

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

Example

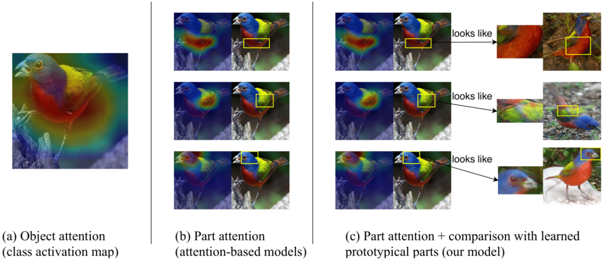


Figure 4: Visual comparison of different types of model interpretability: (a) object-level attention map (e.g., class activation map [56]); (b) part attention (provided by attention-based interpretable models); and (c) part attention with similar prototypical parts (provided by our model).

- 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.

A Template

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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 $\mathrm{expl}(\mathbf{x}, y) \to$ the explanations is 100% **faithful** to the model's decision process.

Take-away

- Gray-box 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)

Alvarez-Melis, D. and Jaakkola, T. S. (2018).
Towards robust interpretability with self-explaining neural networks.
In *Proceedings of the 32nd International Conference on Neural Information Processing Systems*, pages 7786–7795.

Chen, C., Li, O., Tao, D., Barnett, A., Rudin, C., and Su, J. K. (2019).
This looks like that: Deep learning for interpretable image recognition.
Advances in Neural Information Processing Systems, 32:8930–8941.

Li, O., Liu, H., Chen, C., and Rudin, C. (2018).
Deep learning for case-based reasoning through prototypes: A neural network that explains its predictions.
In *Proceedings of the AAAI Conference on Artificial Intelligence*, volume 32.

Lipton, Z. C. (2018).
The mythos of model interpretability: In machine learning, the concept of interpretability is both important and slippery.
Queue, 16(3):31–57.

Snell, J., Swersky, K., and Zemel, R. (2017).
Prototypical networks for few-shot learning.
In *Proceedings of the 31st International Conference on Neural Information Processing Systems*, pages 4080–4090.

Tibshirani, R. (1996).
Regression shrinkage and selection via the lasso.
Journal of the Royal Statistical Society: Series B (Methodological), 58(1):267–288.

Ustun, B. and Rudin, C. (2016).
Supersparse linear integer models for optimized medical scoring systems.
Machine Learning, 102(3):349–391.

Wu, M., Hughes, M. C., Parbhoo, S., Zazzi, M., Roth, V., and Doshi-Velez, F. (2018).
Beyond sparsity: Tree regularization of deep models for interpretability.
In *Thirty-Second AAAI Conference on Artificial Intelligence*.