

CS 4501/6501 Interpretable Machine Learning

Neural Networks and Deep Learning

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Overview

1. What is a white box looks like?
2. What is a neural network?
3. Why we need neural network models?
4. Why neural network is a black box?

What is a white box looks like?

Linear Models

Directly modeling a linear classifier as

$$h_y(\boldsymbol{x}) = \boldsymbol{w}_y^\top \boldsymbol{x} + b_y \quad (1)$$

- ▶ $\boldsymbol{x} \in \mathbb{N}^V$: vector, bag-of-words representation
- ▶ $\boldsymbol{w}_y \in \mathbb{R}^V$: vector, classification weights associated with label y
- ▶ $b_y \in \mathbb{R}$: scalar, label bias in the training set y

Logistic Regression

Rewrite the linear decision function in the log probabilistic form

$$\log P(y | x) \propto \underbrace{\mathbf{w}_y^\top \mathbf{x} + b_y}_{h_y(x)} \quad (2)$$

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To make sure $P(y | x)$ is a valid definition of probability, we need to make sure $\sum_y P(y | x) = 1$,

$$P(\textcolor{red}{y} | x) = \frac{\exp(w_{\textcolor{red}{y}}^\top x + b_{\textcolor{red}{y}})}{\sum_{y' \in \mathcal{Y}} \exp(w_{y'}^\top x + b_{y'})} \quad (4)$$

Alternative Form

Rewriting x and w as

- ▶ $x^\top = [x_1, x_2, \dots, x_V, \mathbf{1}]$
- ▶ $w_y^\top = [w_1, w_2, \dots, w_V, \mathbf{b}_y]$

allows us to have a more concise form

$$P(y \mid x) = \frac{\exp(w_y^\top x)}{\sum_{y' \in \mathcal{Y}} \exp(w_{y'}^\top x)} \quad (5)$$

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Comments:

- ▶ $\frac{\exp(a)}{\sum_{a'} \exp(a')}$ is the **softmax** function
- ▶ This form works with any size of \mathcal{Y} — it does not have to be a binary classification problem.

Binary Classifier

Assume $\mathcal{Y} = \{\text{NEG}, \text{POS}\}$, then the corresponding logistic regression classifier with $Y = \text{Pos}$ is

$$P(Y = \text{Pos} \mid x) = \frac{1}{1 + \exp(-w^\top x)} \quad (6)$$

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- ▶ $P(Y = \text{NEG} \mid \mathbf{x}) = 1 - P(Y = \text{Pos} \mid \mathbf{x})$

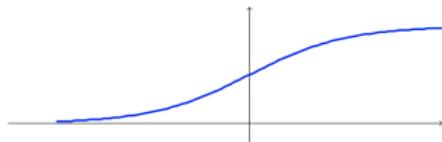
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- ▶ $P(Y = \text{NEG} | \mathbf{x}) = 1 - P(Y = \text{Pos} | \mathbf{x})$
- ▶ $\frac{1}{1+\exp(-z)}$ is the Sigmoid function



Two Questions on Building LR Models

... of building a logistic regression classifier

$$P(y | x) = \frac{\exp(w_y^\top x)}{\sum_{y' \in \mathcal{Y}} \exp(w_{y'}^\top x)} \quad (7)$$

- ▶ How to learn the parameters $W = \{w_y\}_{y \in \mathcal{Y}}$?

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$$P(y | x) = \frac{\exp(w_y^\top x)}{\sum_{y' \in \mathcal{Y}} \exp(w_{y'}^\top x)} \quad (7)$$

- ▶ How to learn the parameters $W = \{w_y\}_{y \in \mathcal{Y}}$?
- ▶ Can x be better than the bag-of-words representations?

Review: (Log)-likelihood Function

With a collection of training examples $\{(x^{(i)}, y^{(i)})\}_{i=1}^m$, the likelihood function of $\{w_y\}_{y \in \mathcal{Y}}$ is

$$L(W) = \prod_{i=1}^m P(y^{(i)} | x^{(i)}) \quad (8)$$

and the **log**-likelihood function is

$$\ell(\{w_y\}) = \sum_{i=1}^m \log P(y^{(i)} | x^{(i)}) \quad (9)$$

Log-likelihood Function of a LR Model

With the definition of a LR model

$$P(y | x) = \frac{\exp(w_y^\top x)}{\sum_{y' \in \mathcal{Y}} \exp(w_{y'}^\top x)} \quad (10)$$

the log-likelihood function is

$$\ell(W) = \sum_{i=1}^m \log P(y^{(i)} | x^{(i)}) \quad (11)$$

$$= \sum_{i=1}^m \left\{ w_{y^{(i)}}^\top x^{(i)} - \log \sum_{y' \in \mathcal{Y}} \exp(w_{y'}^\top x^{(i)}) \right\} \quad (12)$$

Given the training examples $\{(x^{(i)}, y^{(i)})\}_{i=1}^m$, $\ell(W)$ is a **function of** $W = \{w_y\}$.

Optimization with Gradient

MLE is equivalent to **minimize** the Negative Log-Likelihood (NLL) as

$$\begin{aligned}\text{NLL}(W) &= -\ell(W) \\ &= \sum_{i=1}^m \left\{ -w_{y^{(i)}}^\top x^{(i)} + \log \sum_{y' \in \mathcal{Y}} \exp(w_{y'}^\top x) \right\}\end{aligned}$$

then, the parameter w_y associated with label y can be updated as

$$w_y \leftarrow w_y - \eta \cdot \frac{\partial \text{NLL}(\{w_y\})}{\partial w_y}, \quad \forall y \in \mathcal{Y} \quad (13)$$

where η is called **learning rate**.

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Two questions answered by the update equation

- (1) which direction?
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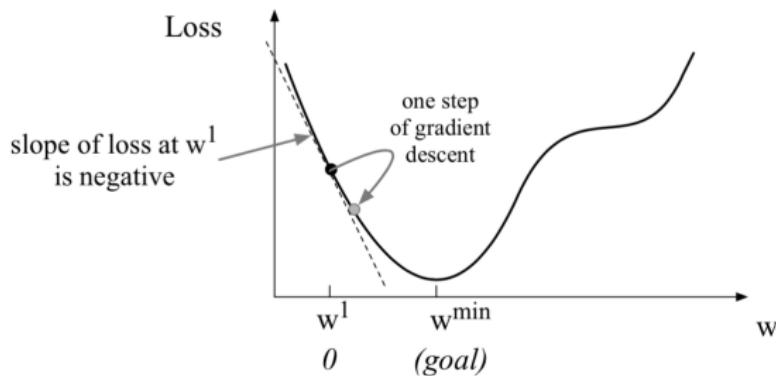
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Training Procedure

Steps for parameter estimation, given the current parameter $\{w_y\}$

1. Compute the derivative

$$\frac{\partial \text{NLL}(\{w_y\})}{\partial w_y}, \quad \forall y \in \mathcal{Y}$$

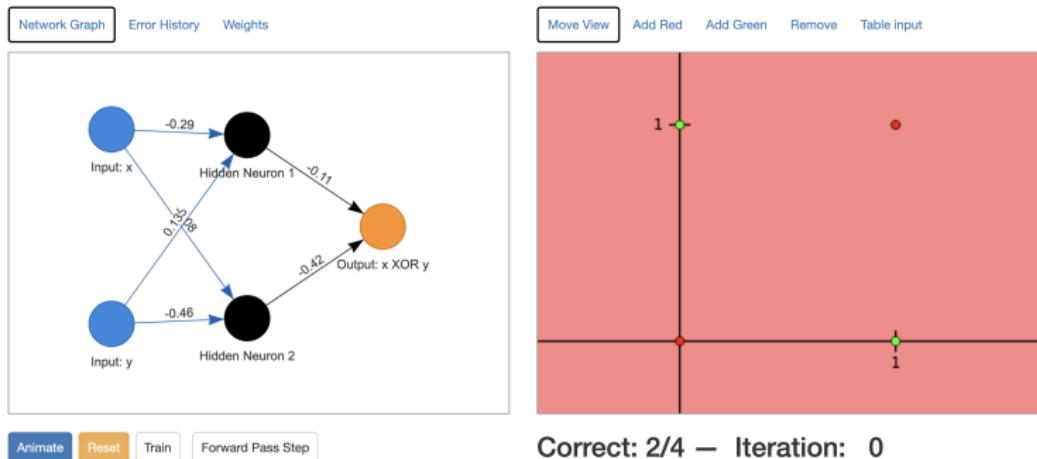
2. Update parameters with

$$w_y \leftarrow w_y - \eta \cdot \frac{\partial \text{NLL}(\{w_y\})}{\partial w_y}, \quad \forall y \in \mathcal{Y}$$

3. If not **done**, return to step 1

Neural Network Demo

A simple demo with 2-dimensional inputs



<https://phiresky.github.io/neural-network-demo/>

Sentiment Classification

A few training examples from Yelp Review

Label	Text
5	Love the staff, love the meat, love the place. Prepare for a long line around lunch or dinner hours ...
5	Super simple place but amazing nonetheless. It's been around since the 30's and they still serve the same thing ...

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1	Actually I would like to give them a big fat zero. Any vet's office that would tell ...

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1	Actually I would like to give them a big fat zero. Any vet's office that would tell ...
2	OK so first off the the burger was great as far as the taste. But I got super sick after eating it ...

Classification Configuration and Performance

Vocabulary size	17,490
Training size	40K
Development size	5K
Classifier	Logistic regression
Regularization parameter	$C = 1$
Training accuracy	88.48%
Development accuracy	61.22%

You can find the demo code via the [link](#)

Interpretability: Global

RATING	FEATURES
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4	default hankering drawback bojangles pleasantly hazel- nut customize gratuity excellent tremendously
5	phenomenal incredible amazing gem excellent pleas- antly hesitate master magnificent spotless

Interpretability: Local

The prediction on the following is 5

I love the service here , they ' re on it !

After pre-processing, we remove the high-frequency word I and the punctuation

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FEATURE	CLASSIFICATION WEIGHT
love	0.85
service	0.04
on	0.01
they	-0.00
it	-0.02
the	-0.06
re	-0.13
here	-0.15

What is a neural network?

Logistic Regression

- ▶ An unified form for $y \in \{-1, +1\}$

$$p(Y = +1 \mid \mathbf{x}) = \frac{1}{1 + \exp(-\langle \mathbf{w}, \mathbf{x} \rangle)} \quad (15)$$

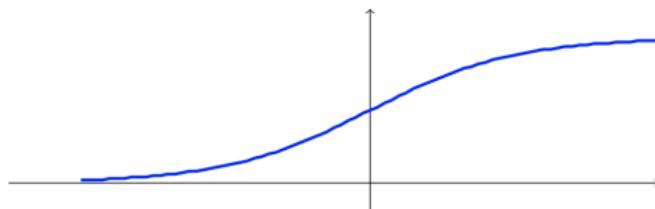
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$$p(Y = +1 | \mathbf{x}) = \frac{1}{1 + \exp(-\langle \mathbf{w}, \mathbf{x} \rangle)} \quad (15)$$

- ▶ The sigmoid function $\sigma(a)$ with $a \in \mathbb{R}$

$$\sigma(a) = \frac{1}{1 + \exp(-a)} \quad (16)$$

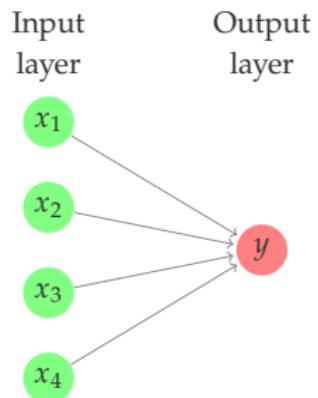


Graphical Representation

- ▶ A specific example of LR

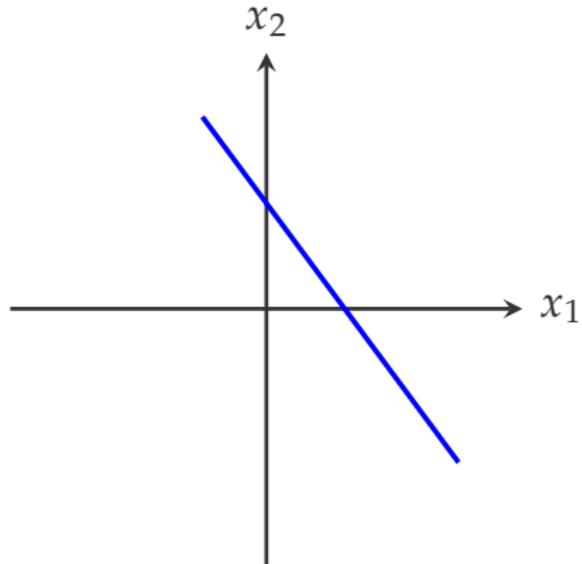
$$p(Y = 1 \mid \boldsymbol{x}) = \sigma\left(\sum_{j=1}^4 w_j x_{\cdot j}\right) \quad (17)$$

- ▶ The graphical representation of this LR model is



Capacity of a LR

Logistic regression gives a linear decision boundary



From LR to Neural Networks

Build upon logistic regression, a simple neural network can be constructed as

$$z_k = \sigma\left(\sum_{j=1}^d w_{k,j}^{(1)} x_{\cdot,j}\right) \quad k \in [K] \quad (18)$$

$$P(y = 1 \mid x) = \sigma\left(\sum_{k=1}^K w_k^{(o)} z_k\right) \quad (19)$$

- ▶ $x \in \mathbb{R}^d$: d -dimensional input
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- ▶ $x \in \mathbb{R}^d$: d -dimensional input
- ▶ $y \in \{-1, +1\}$ (binary classification problem)
- ▶ $\{w_{k,i}^{(1)}\}$ and $\{w_k^{(o)}\}$ are two sets of the parameters, and
- ▶ K is the number of hidden units, each of them has the same form as a LR.

Mathematical Formulation

- ▶ Element-wise formulation

$$z_k = \sigma\left(\sum_{j=1}^d w_{k,j}^{(1)} x_{\cdot,j}\right) \quad k \in [K] \quad (20)$$

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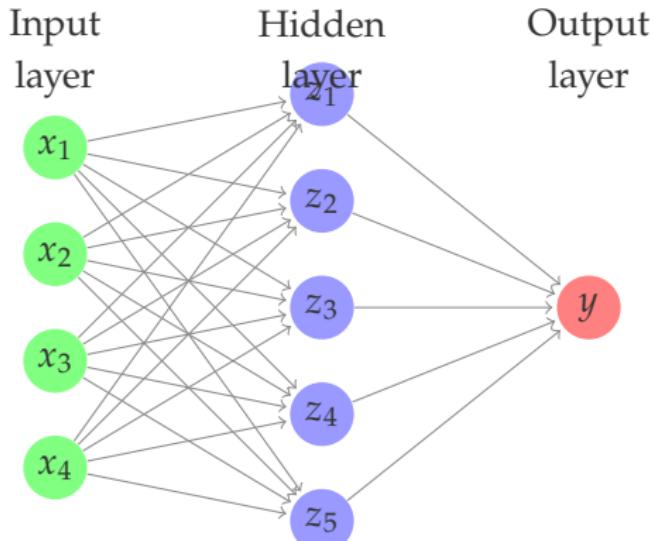
- ▶ Matrix-vector formulation

$$z = \sigma(\mathbf{W}^{(1)} \mathbf{x}) \quad (22)$$

$$P(y = +1 \mid x) = \sigma((\mathbf{w}^{(o)})^\top z) \quad (23)$$

where $\mathbf{W}^{(1)} \in \mathbb{R}^{K \times d}$ and $\mathbf{w}^{(o)} \in \mathbb{R}^K$

Graphical Representation

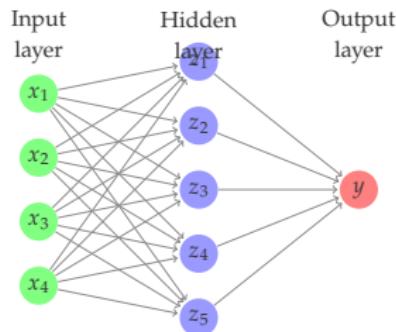


- ▶ Depth: 2 (two-layer neural network)
- ▶ Width: 5 (the maximal number of units in each layer)

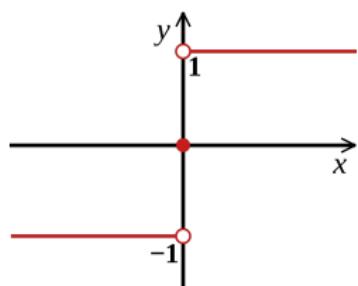
Hypothesis Space

The hypothesis space of neural networks is usually defined by the **architecture** of the network, which includes

- ▶ the nodes in the network,
- ▶ the connections in the network, and
- ▶ the **activation function** (e.g., σ)

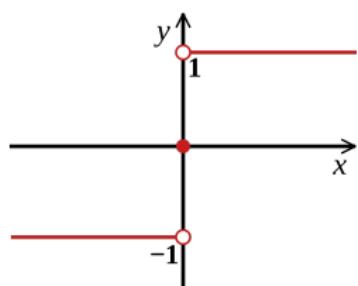


Other Activation Functions

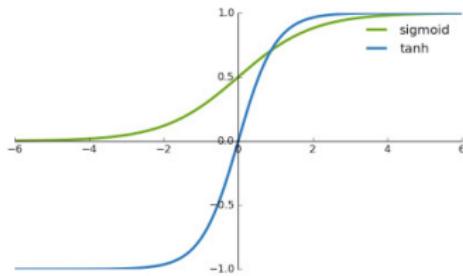


(a) Sign function

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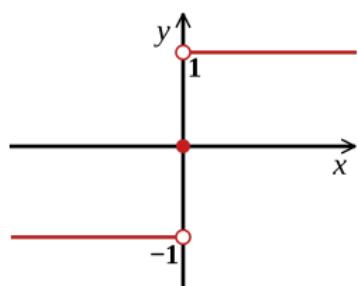


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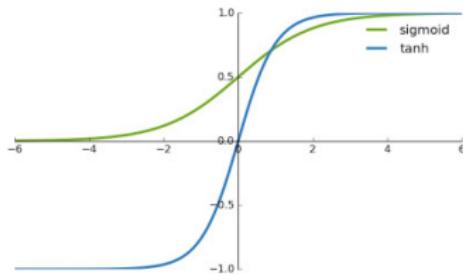


(b) Tanh function

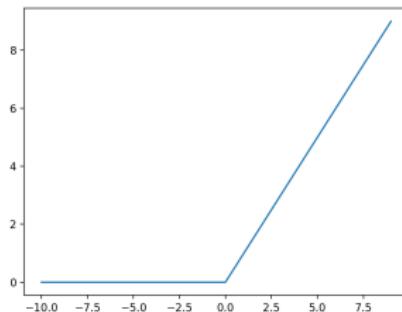
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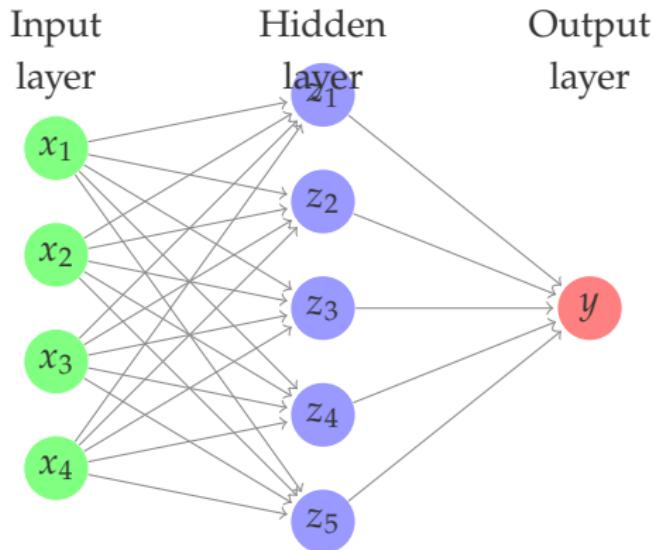


(c) ReLU function
[Jarrett et al., 2009]

Network Architecture

We are going to build a simple neural network for text classification.
It includes three layers as the previous example

- ▶ Input layer
- ▶ Hidden layer
- ▶ Output layer



Example

Consider the following special case, where we have a 4-dimensional BoW representation $x \in \mathbb{R}^4$ and a weight matrix $W \in \mathbb{R}^{5 \times 4}$

$$Wx = \begin{bmatrix} 0.1 & 0.3 & 0.7 & 0.9 \\ 0.2 & 0.8 & 0.3 & 0.5 \\ 0.4 & 0.8 & 0.6 & 0.1 \\ 0.7 & 0.2 & 0.9 & 0.2 \\ 0.4 & 0.5 & 0.8 & 0.9 \end{bmatrix} \cdot \begin{bmatrix} 0 \\ 1 \\ 0 \\ 1 \end{bmatrix} \quad (24)$$

(25)

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$$= \begin{bmatrix} 0.3 \\ 0.8 \\ 0.8 \\ 0.2 \\ 0.5 \end{bmatrix} + \begin{bmatrix} 0.9 \\ 0.5 \\ 0.1 \\ 0.2 \\ 0.9 \end{bmatrix} \quad (25)$$

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- ▶ Each column vector in W corresponds one word in the BoW representation
- ▶ The column vectors can be considered as representations of words, in other words, *word embeddings*

Data Processing

Similar to building a logistic regression classifier, we need the following steps in data processing

- ▶ Tokenize texts
- ▶ Build a vocab
- ▶ Convert a text into a collection of word indices (instead of using BoW representations)

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In addition, we also need to divide the whole set of texts into small batches

- ▶ Create mini-batches

Output Layer

For the same text classification task, we use the following configuration:

- ▶ Input dimension: $x \in \mathbb{R}^{17K}$
- ▶ Hidden layer: $h \in \mathbb{R}^{32}$
- ▶ Output layer: $y \in \{1, \dots, 5\}$

You can find an extremely simple implementation via the same link, the dev accuracy is 65%

Why we need neural network models?

Distributed Representation

- ▶ Bag-of-words representations

VOCAB	coffee	love	like	...	tea	you
love	(0	1	0	...	0	0)

¹I made up those numbers for illustration purpose

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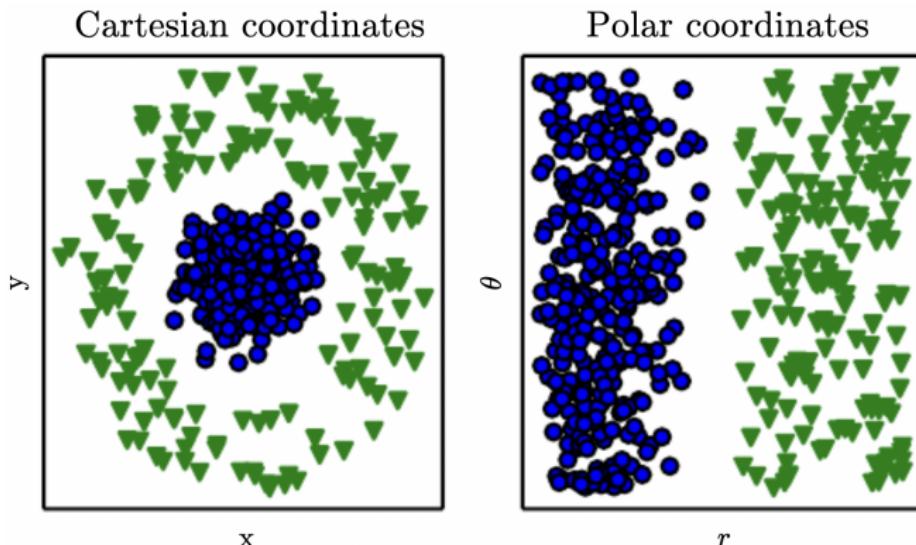
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- ▶ Distributed representations allow simple algebraic operations for semantic meanings
 - ▶ E.g., the cosine value between two word embeddings measures their semantic similarity

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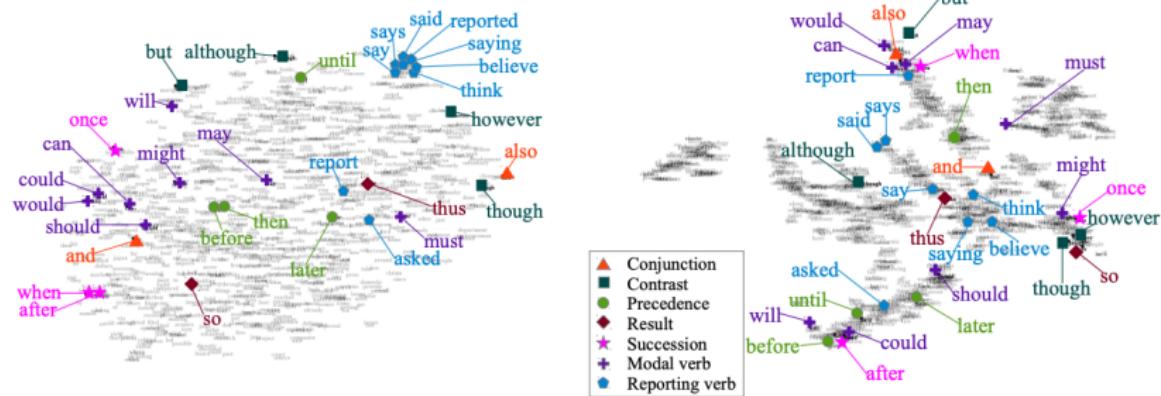
The Value of Different Representations

Different representations lead to different levels of challenge in machine learning



Advantage of Representation Learning

Driven by supervision signals, the model can learn some task-specific information and encode in word embeddings



Similar advantage exists in any other supervised learning tasks
[Bengio et al., 2013]

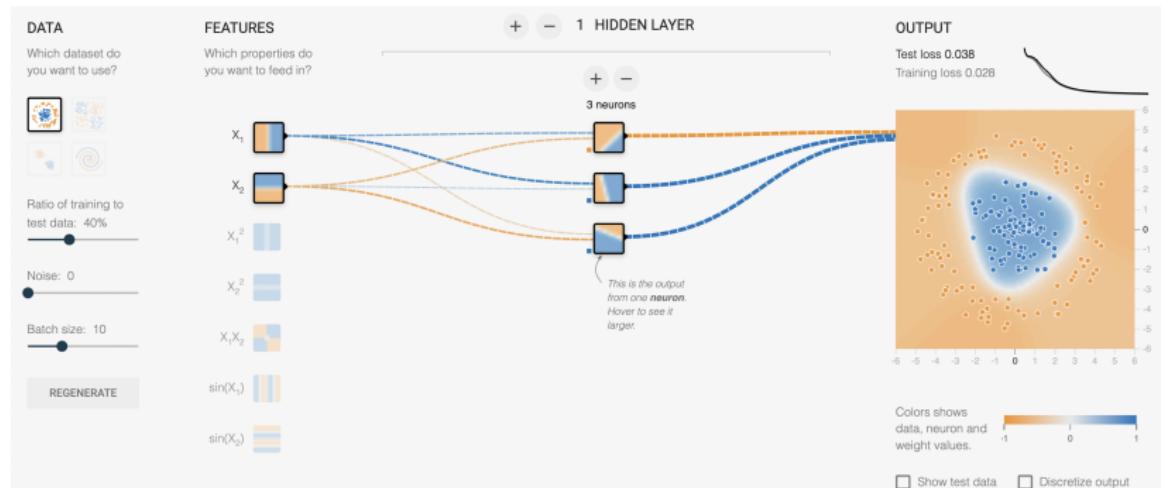
Neural Network as Universal Approximators

Neural network as universal approximators

- ▶ With arbitrary width and bounded depth [Cybenko, 1989]
- ▶ With arbitrary depth and limited width [Kidger and Lyons, 2020]

Model Capacity via Function Composition

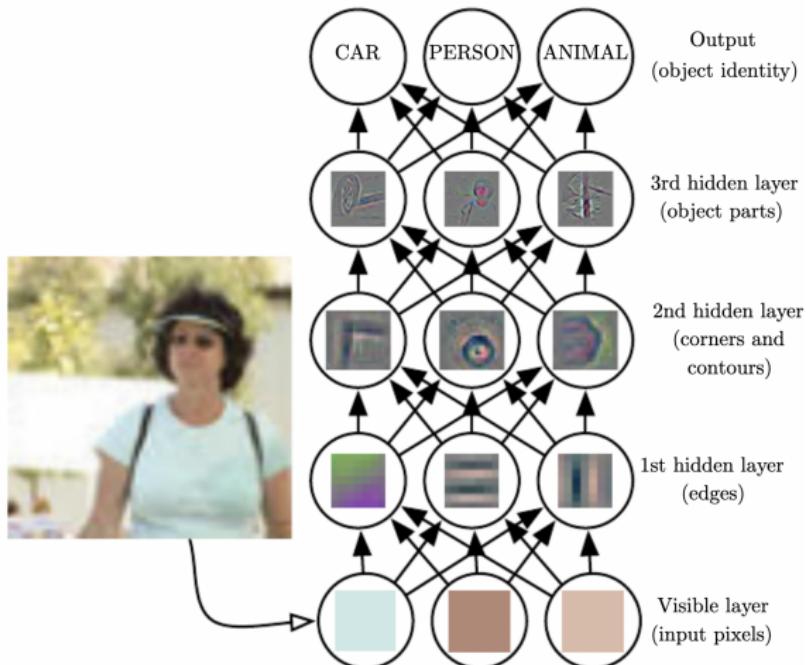
A Toy Example about Function Composition:



<https://playground.tensorflow.org/>

Model Capacity via Function Composition

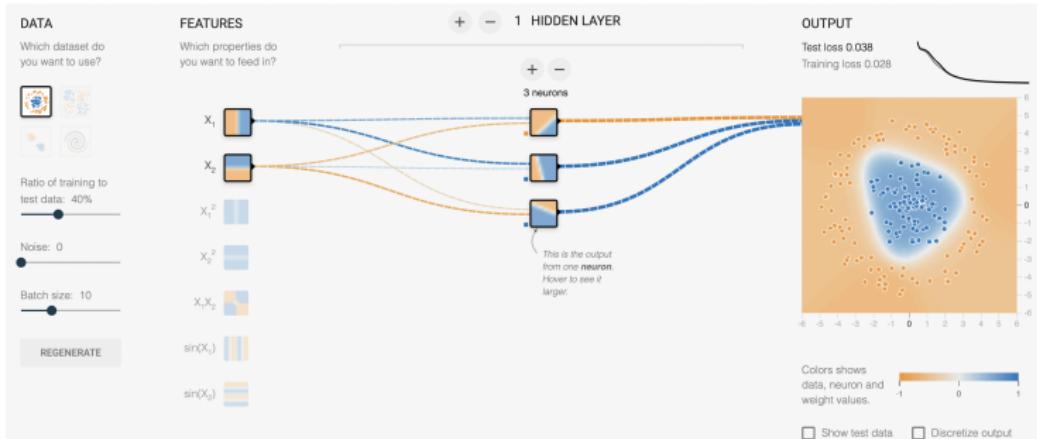
An example of function composition to extract high-level features



Why neural network is a black
box?

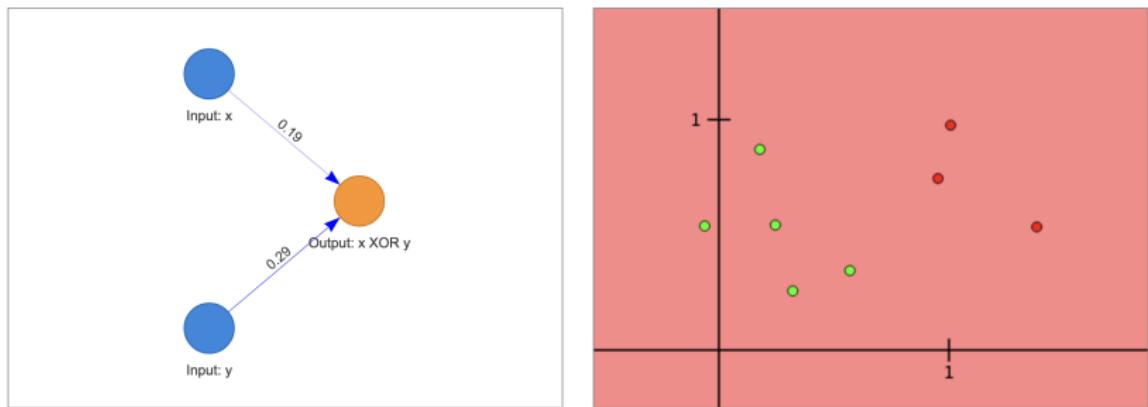
Is Neural Network a Black Box?

Not exactly, we can analyze what it learns when the model is small



Example

Model interpretability: model predictions can be interpreted as *certain* rules associated with inputs²

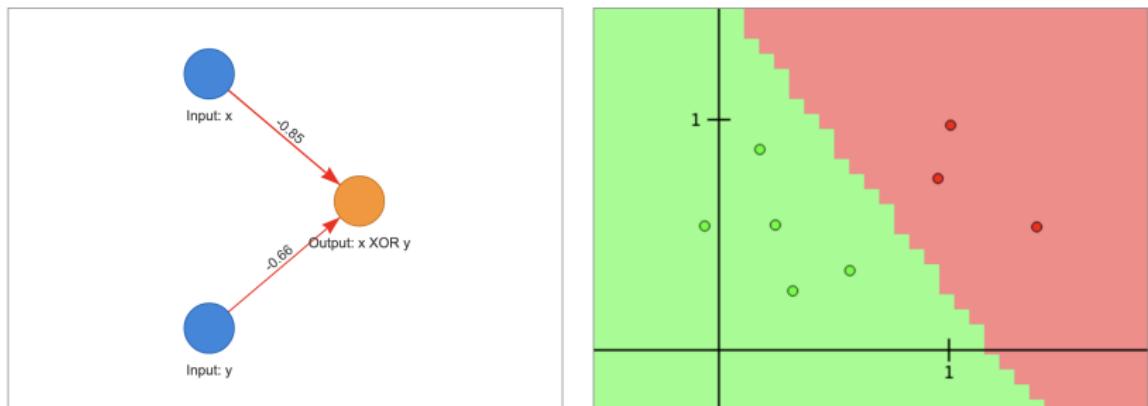


This is equivalent to a logistic regression model

²This is by no means a formal definition of interpretability

Example

Model interpretability: model predictions can be interpreted as *certain rules associated with inputs*²

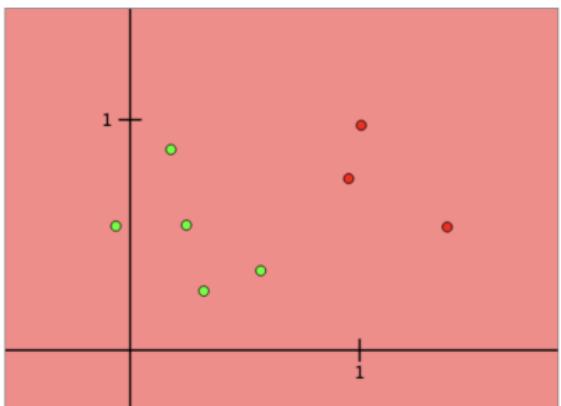
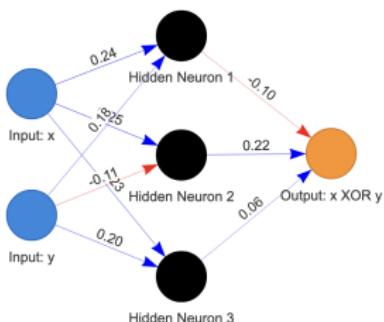


This is equivalent to a logistic regression model

²This is by no means a formal definition of interpretability

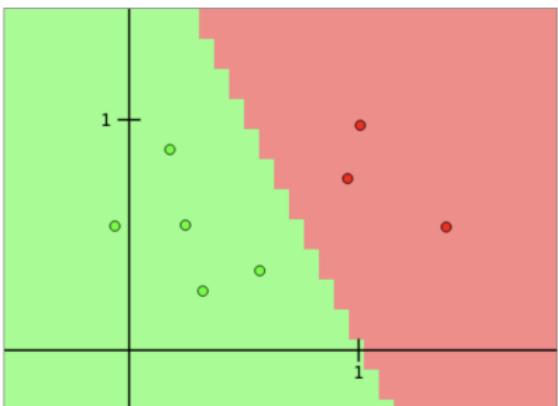
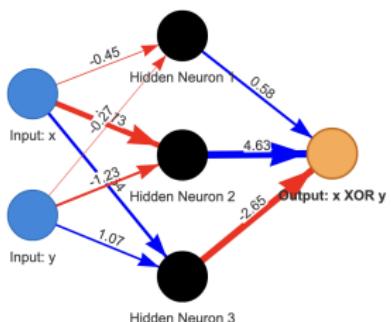
With a Simple Neural Network

With randomly initialized weights (classifying all examples as negative), the neural network (with one hidden layer) can easily learn a classifier with 100%



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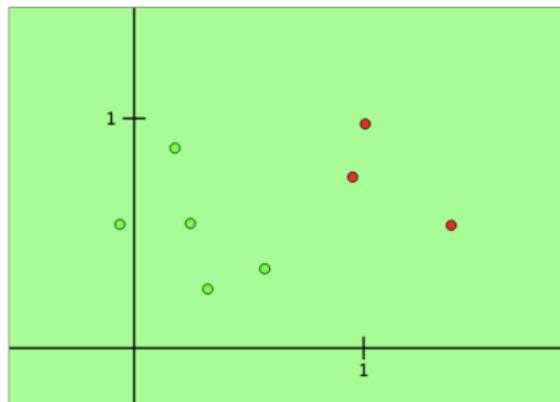
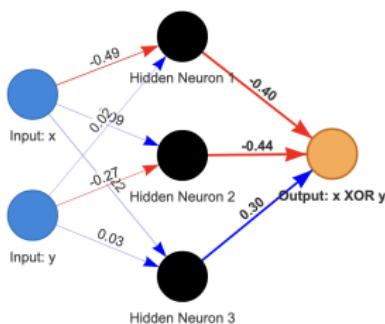
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With the visualization, it is not difficult to identify the second and the third neurons are important.

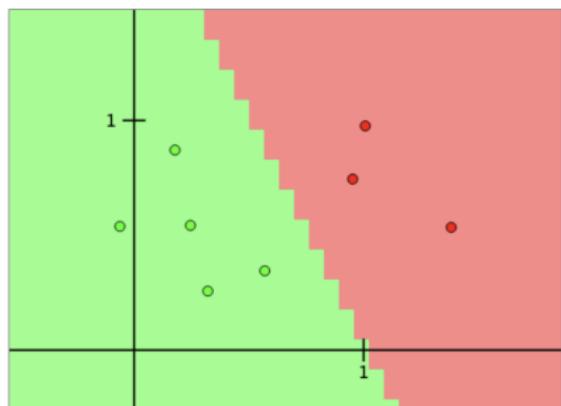
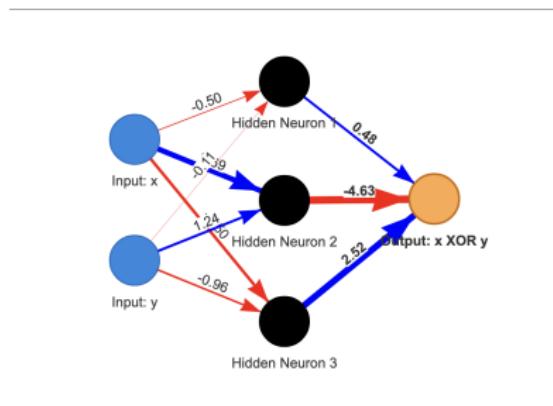
Distributed Representations (II)

With another set of randomly initialized weights (classifying all examples as negative), the learned classifier gives a very similar decision boundary



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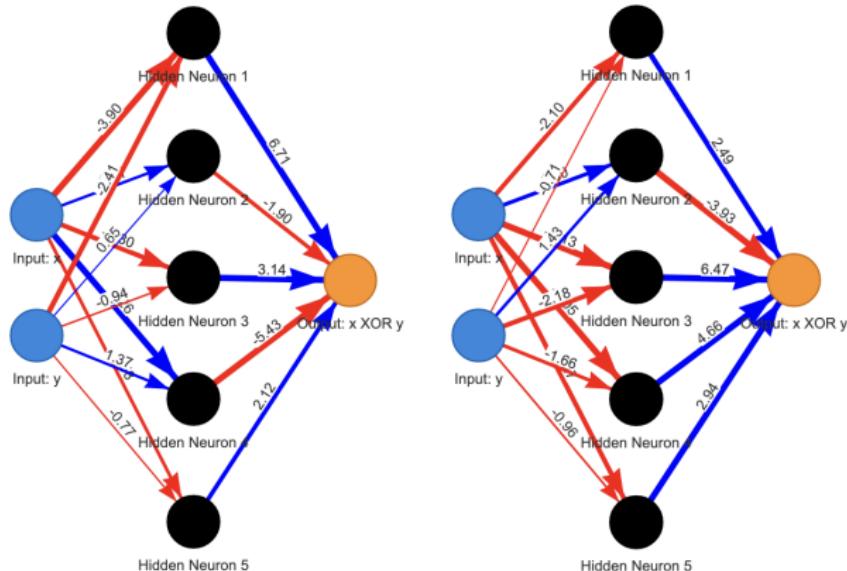
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- ▶ The contributions of the second and third neurons from the these two neural networks are contradicted with each other

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- ▶ The contributions of the second and third neurons from the these two neural networks are contradicted with each other
- ▶ Actually, it is still explainable, if we also consider the contribution from the previous layer

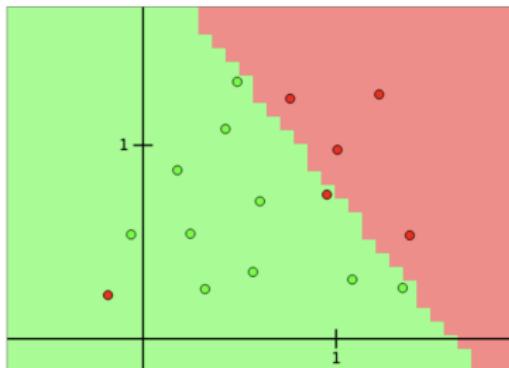
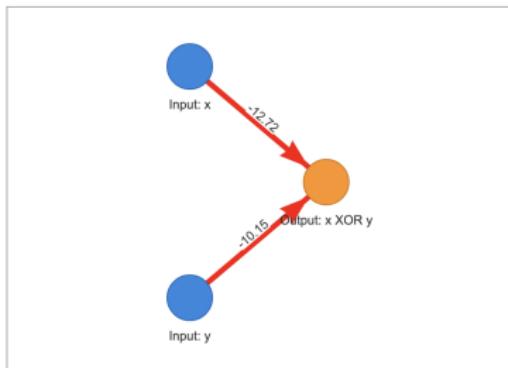
Try to Explain the Following Two Models?



- ▶ The neural network has more parameters than the task actually needs
- ▶ The contributions of hidden neurons are *randomly* distributed

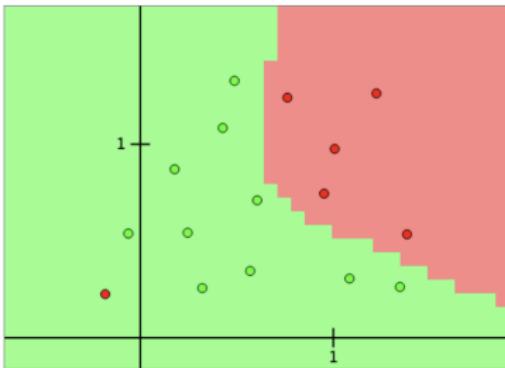
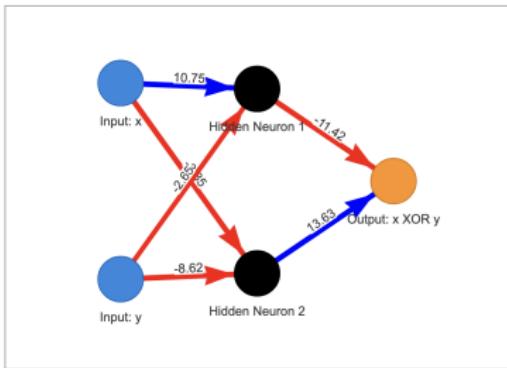
Number of Layers

Similar challenge for interpreting the contributions when we increase the number of layers



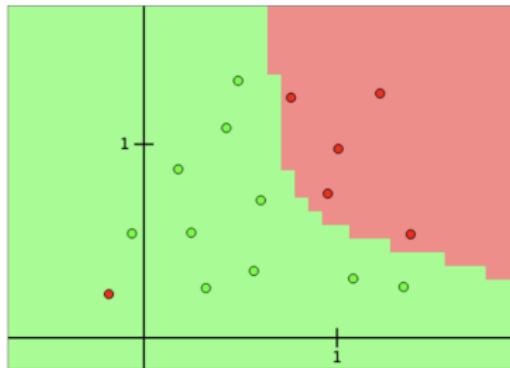
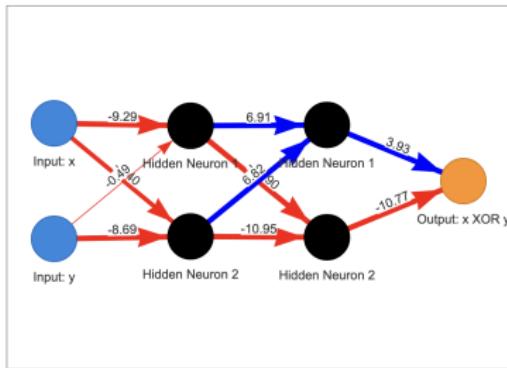
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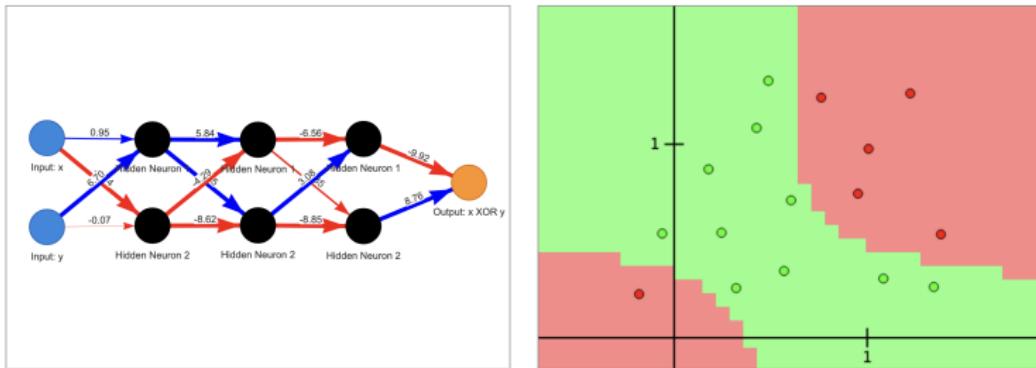
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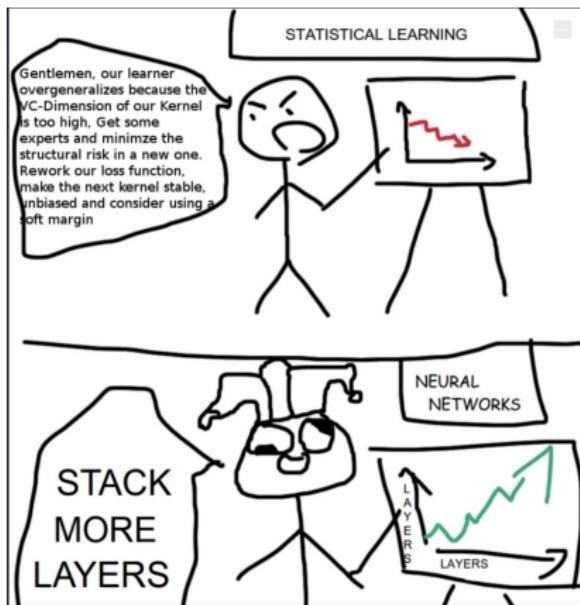
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Similar challenge for interpreting the contributions when we increase the number of layers



Question

Can we train a neural network that maintains good performance and
is also interpretable?

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