# 10-301/601: Introduction to Machine Learning Lecture 11 – Neural Networks

Matt Gormley & Henry Chai

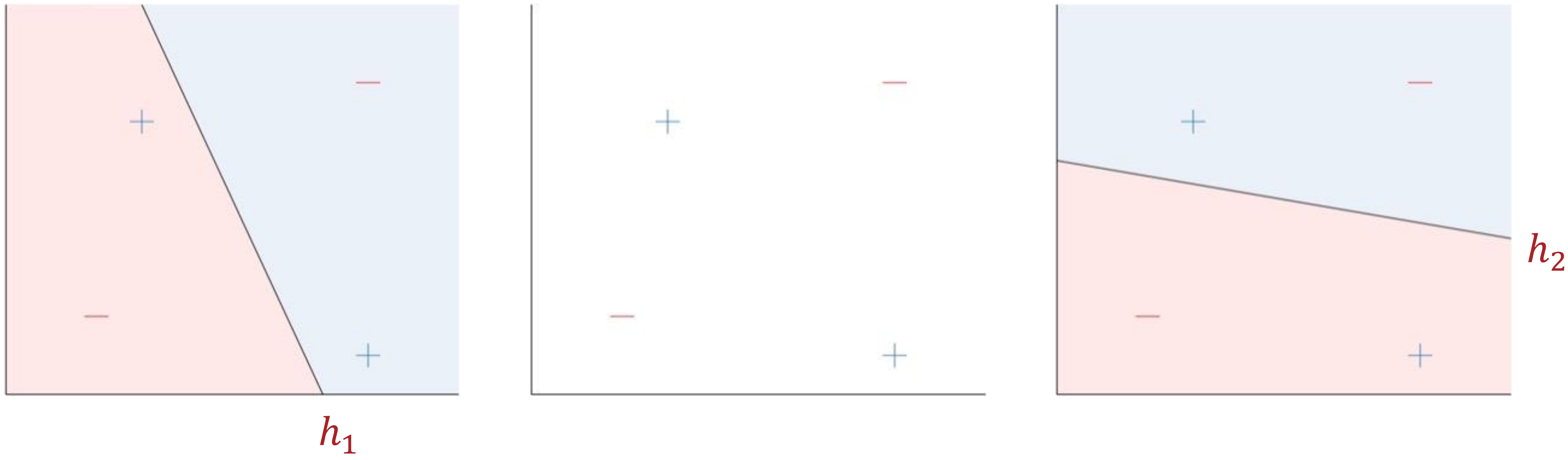
9/30/24

# Front Matter

- Announcements
  - Exam 1 on 9/30 (today!) from 6:30 PM - 8:30 PM
    - Make sure you check the seating chart (on Piazza) so that you know where you're going tonight!
  - Homework 4 released 9/30 (today!), due 10/9 at 11:59 PM

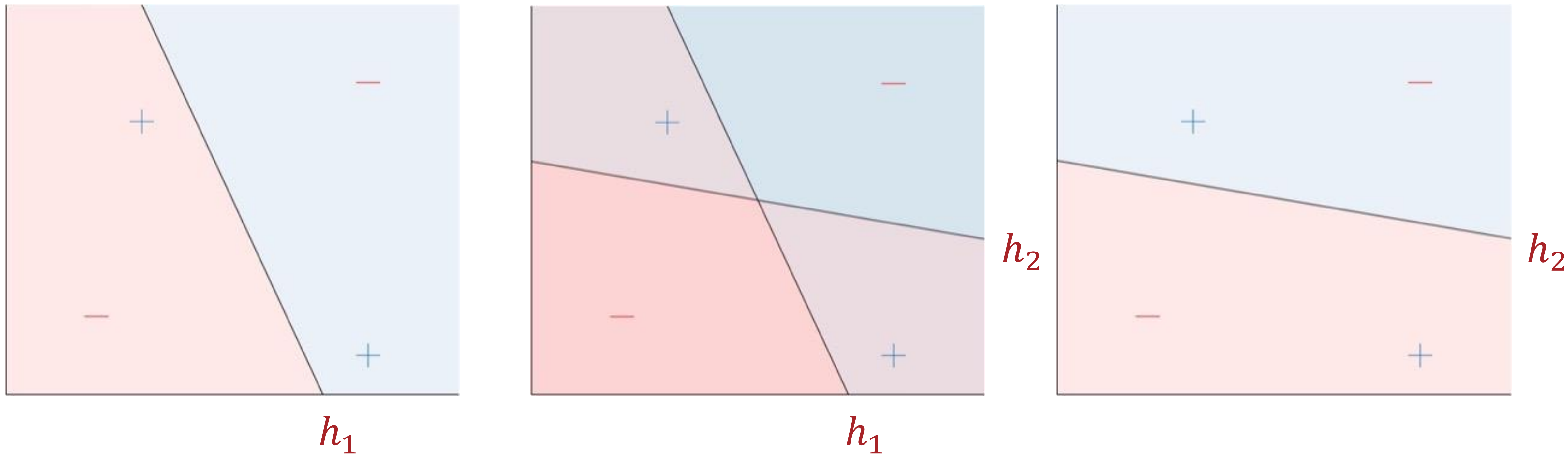
# Biological Neural Network

Source: https://science-art.com/image/?id=2971&m=168&pagename=neural_network_3d#.W_wrzJNKhUM

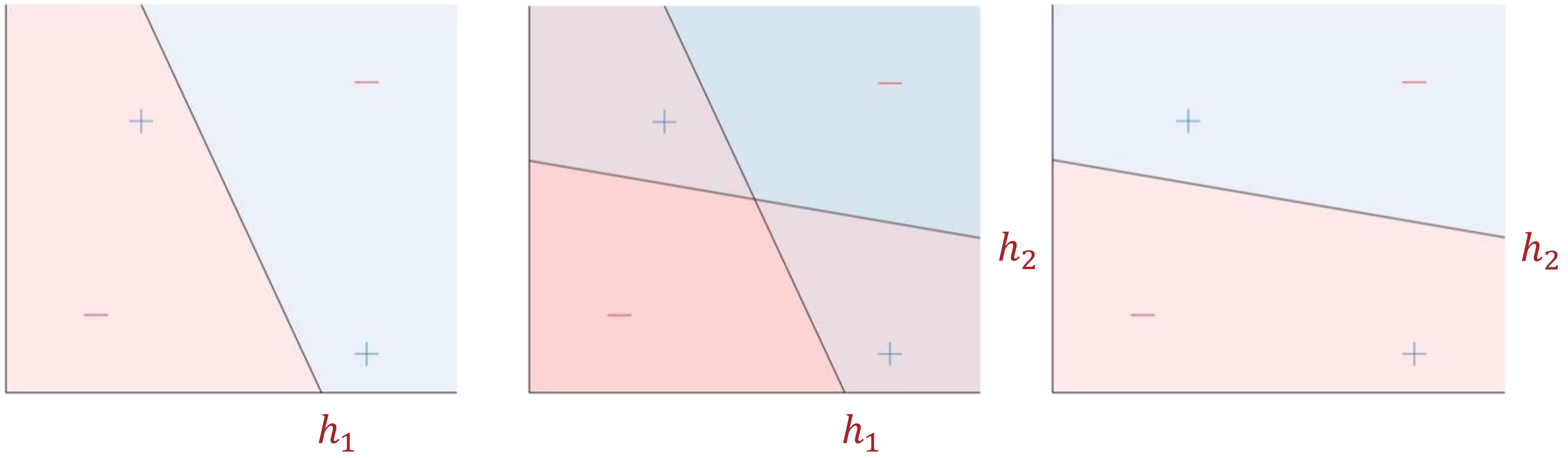



# Perceptrons

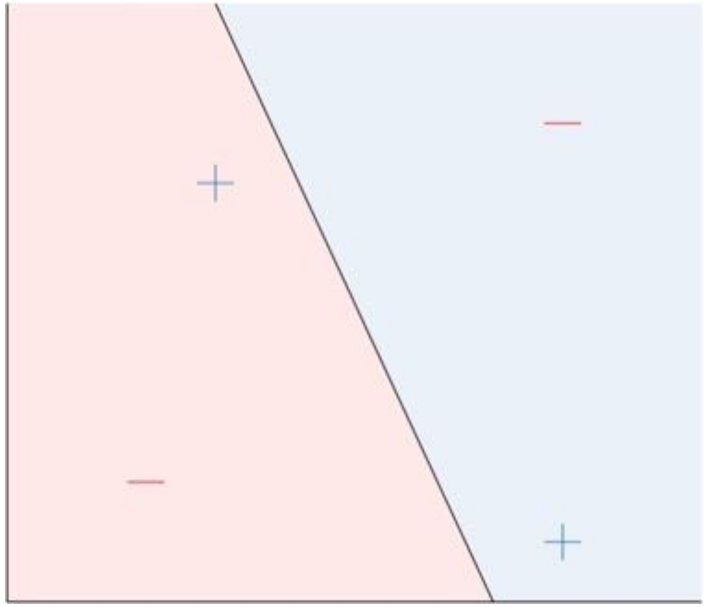
- Linear model for classification
- $h(\boldsymbol{x}) = \operatorname{sign}(\boldsymbol{w}^T \boldsymbol{x})$
- Predictions are $+1$ or $-1$

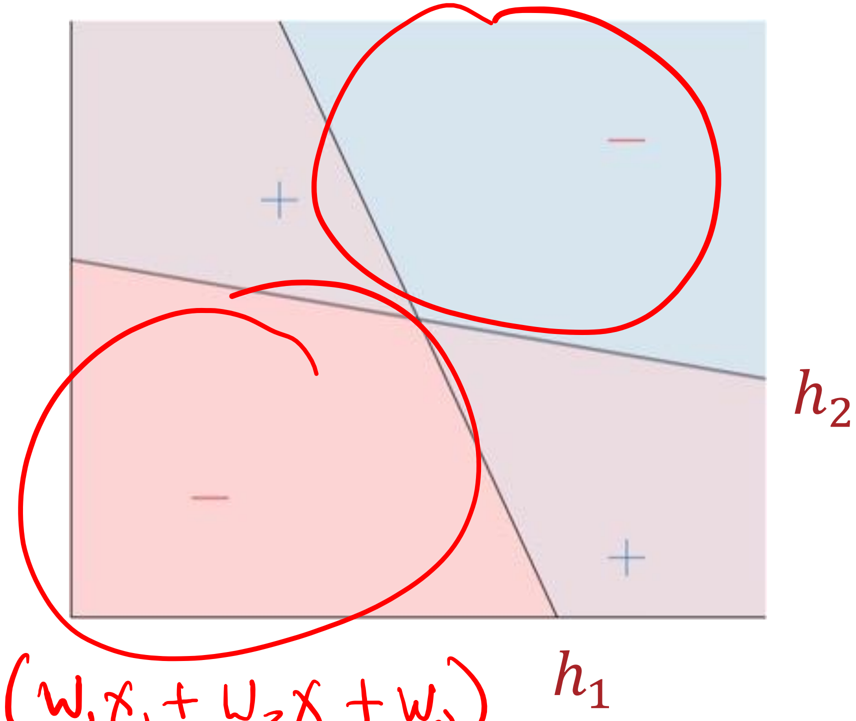



# Combining Perceptrons

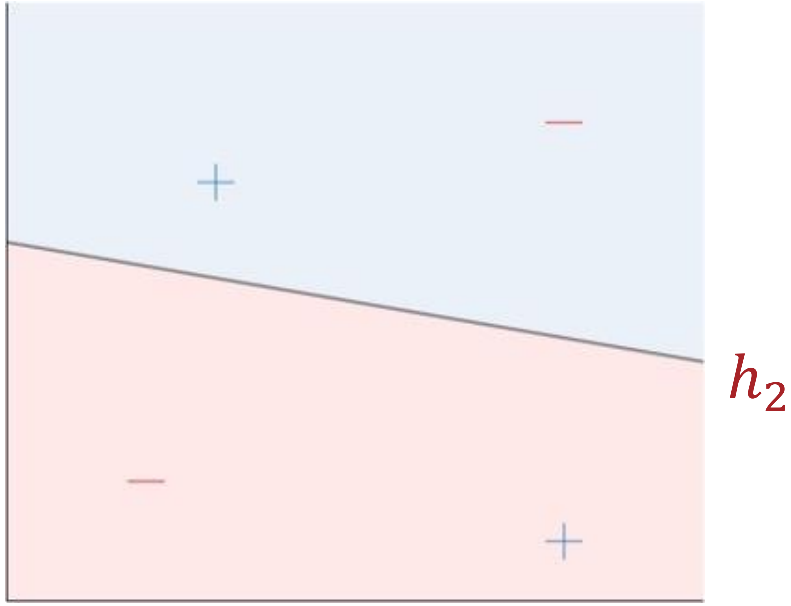



$$h(\boldsymbol{x}) = \begin{cases} +1 \text{ if } (h_1(\boldsymbol{x}) = +1 \text{ and } h_2(\boldsymbol{x}) = -1) \text{ or } (h_1(\boldsymbol{x}) = -1 \text{ and } h_2(\boldsymbol{x}) = +1) \\ -1 \text{ otherwise} \end{cases}$$




$h_1 = \mathrm{sign}(w_1 x_1 + w_2 x_2 + w_0)$




$$h(\boldsymbol{x}) = OR\left(AND\left(h_1(\boldsymbol{x}), \neg h_2(\boldsymbol{x})\right), AND(\neg h_1(\boldsymbol{x}), h_2(\boldsymbol{x}))\right)$$

# Boolean Algebra

- Boolean variables are either $+1$ ("true") or $-1$ ("false")
- Basic Boolean operations:
  - Negation: $\neg z = -1 * z$
  - And: $AND(z_1, z_2) = \begin{cases} +1 \text{ if both } z_1 \text{ and } z_2 \text{ equal } +1 \\ -1 \text{ otherwise} \end{cases}$
  - Or: $OR(z_1, z_2) = \begin{cases} +1 \text{ if either } z_1 \text{ or } z_2 \text{ equals } +1 \\ -1 \text{ otherwise} \end{cases}$

# Boolean Algebra

- Boolean variables are either $+1$ (”true”) or $-1$ (“false”)
- Basic Boolean operations
  - Negation: $\neg z = -1 * z$
  - And: $AND(z_1, z_2) = \text{sign}(z_1 + z_2 - 1.5)$
  - Or: $OR(z_1, z_2) = \text{sign}(z_1 + z_2 + 1.5)$

# Boolean Algebra

- Boolean variables are either $+1$ (”true”) or $-1$ (“false”)
- Basic Boolean operations
  - Negation: $\neg z = -1 * z$
  - And: $AND(z_1, z_2) = \text{sign}\left([-1.5, 1, 1]\begin{bmatrix}1\\z_1\\z_2\end{bmatrix}\right)$
  - Or: $OR(z_1, z_2) = \text{sign}\left([1.5, 1, 1]\begin{bmatrix}1\\z_1\\z_2\end{bmatrix}\right)$

# Building a Network

$$h(\boldsymbol{x}) = OR\left(AND\left(h_1(\boldsymbol{x}), \neg h_2(\boldsymbol{x})\right), AND\left(\neg h_1(\boldsymbol{x}), h_2(\boldsymbol{x})\right)\right)$$

# Building a Network

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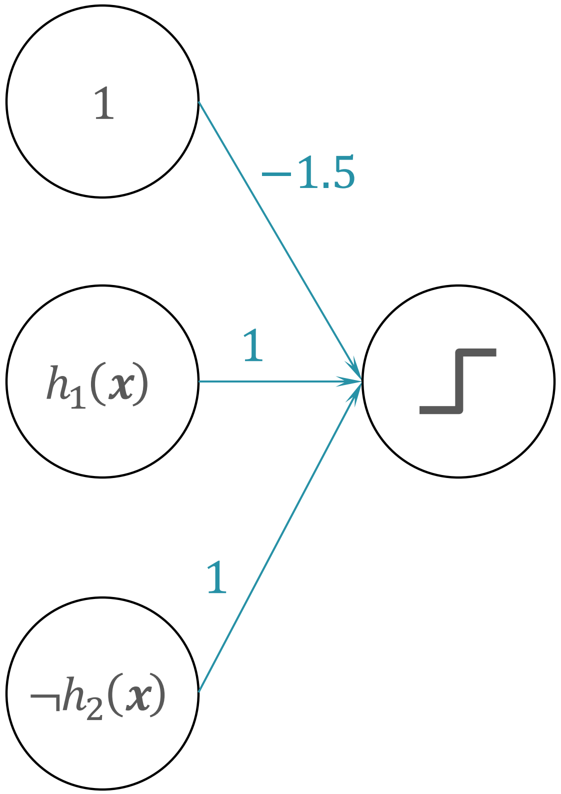

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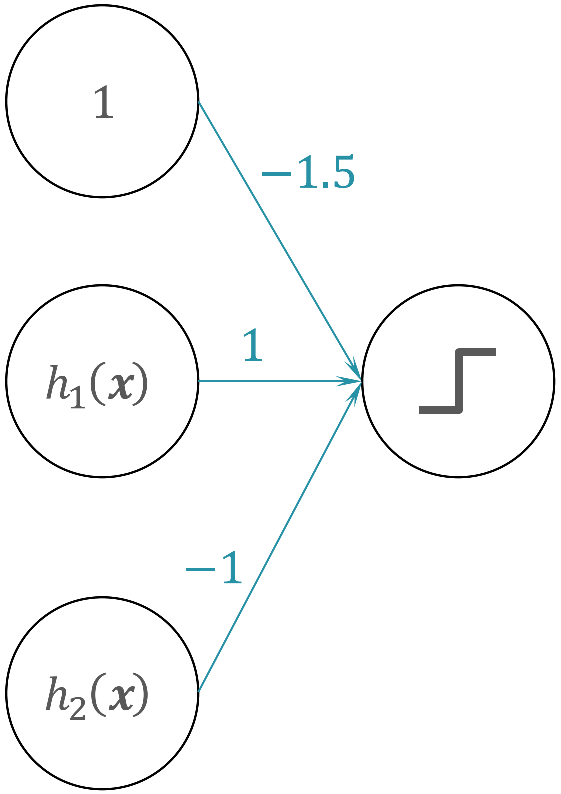

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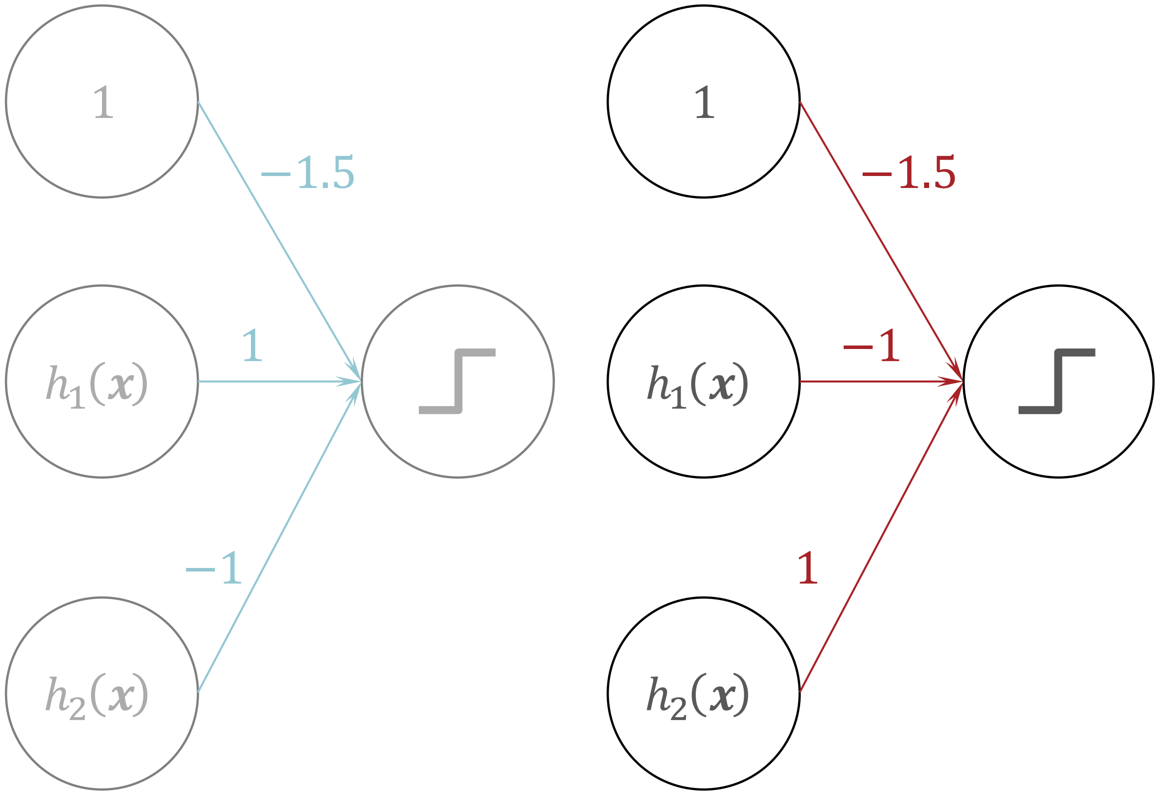

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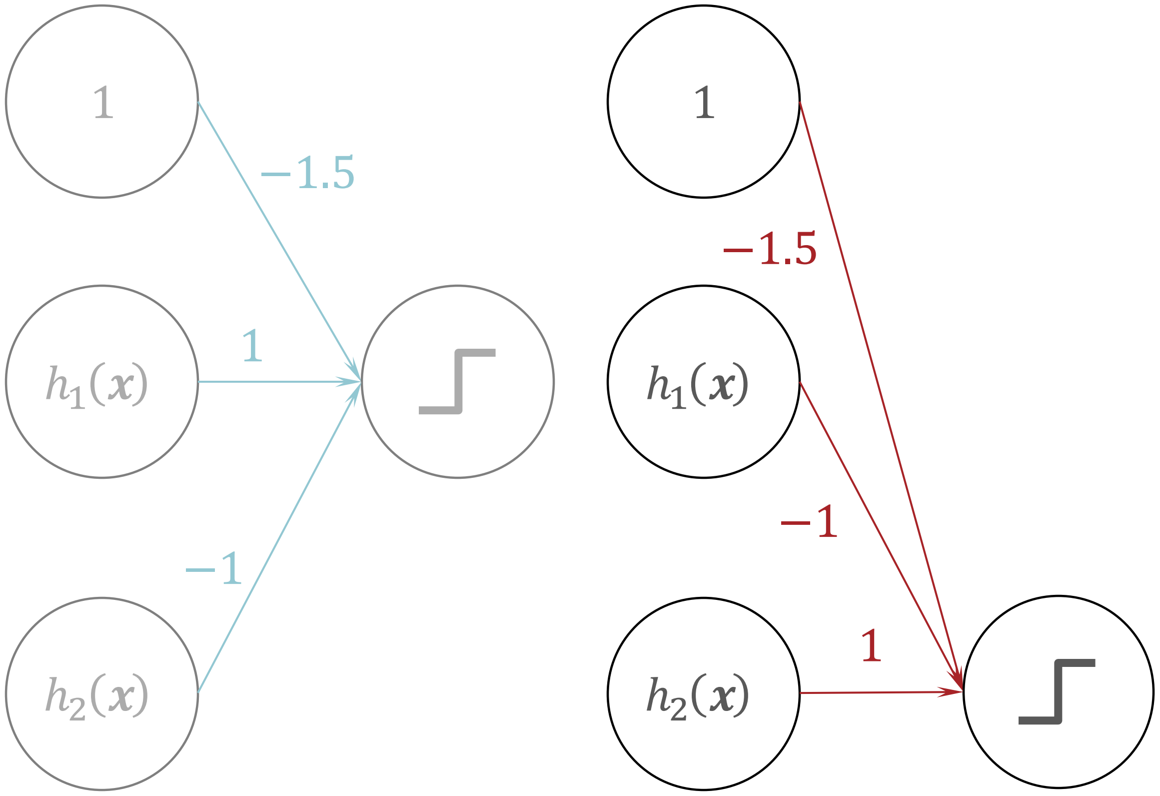

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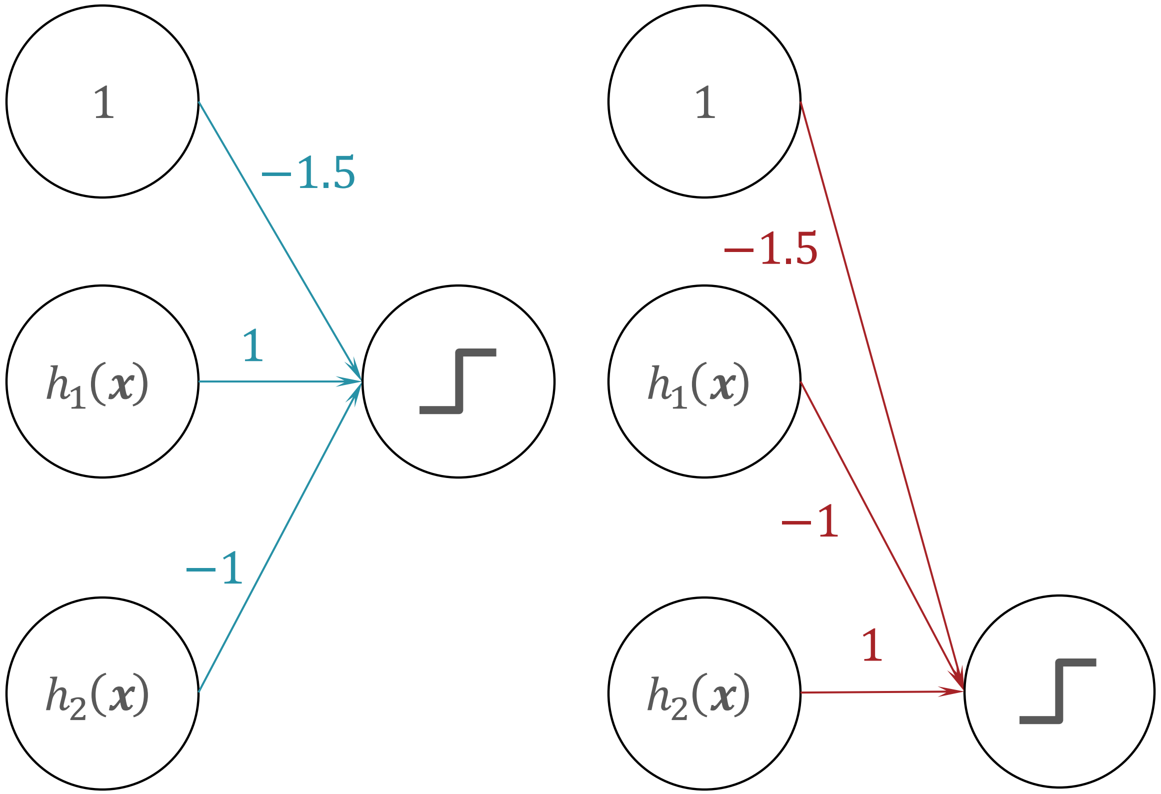

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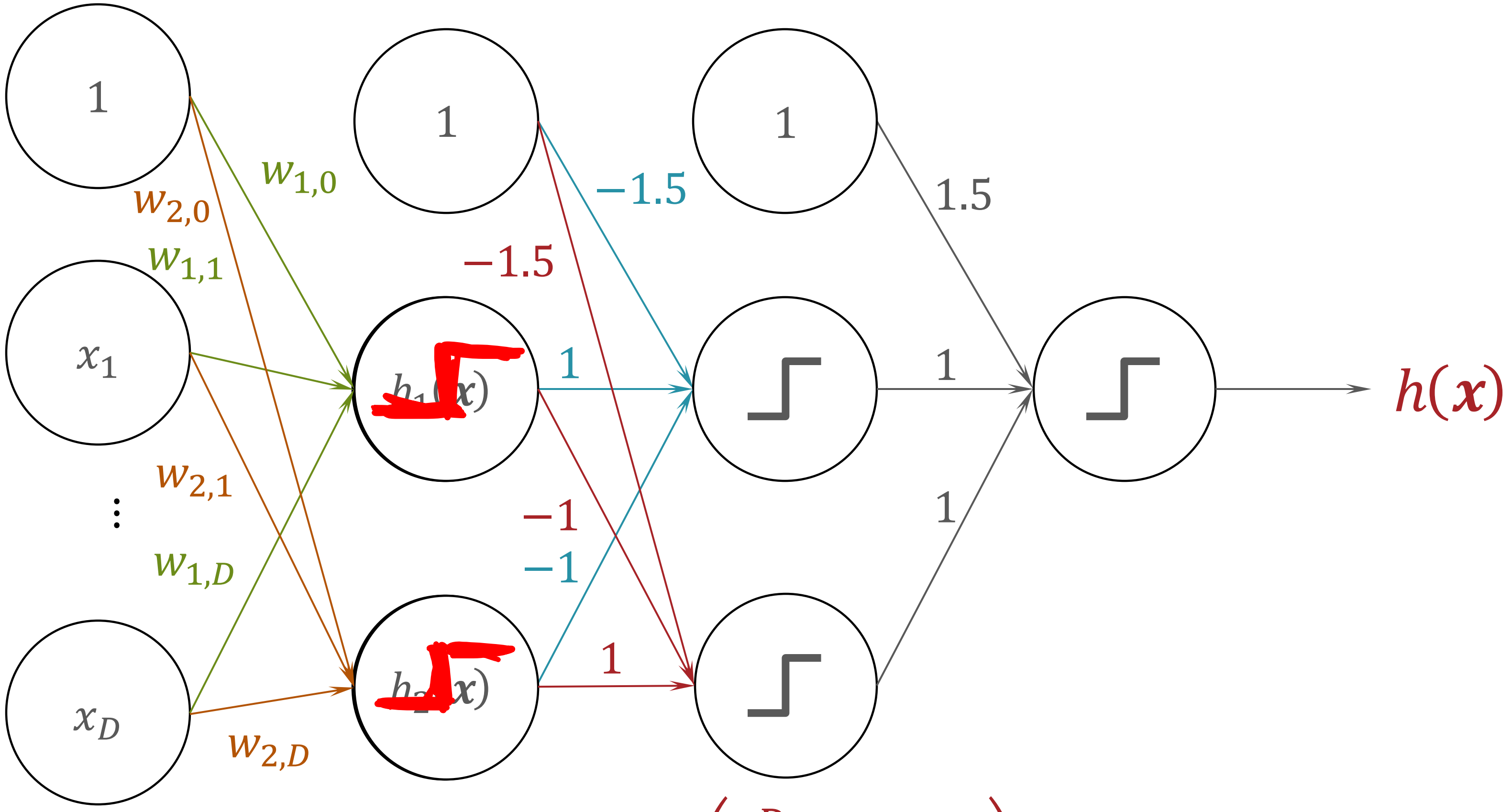


$$h_i(\boldsymbol{x}) = \operatorname{sign}\left(\boldsymbol{w}_i^T \boldsymbol{x}\right) = \operatorname{sign}\left(\sum_{d=0}^{D} w_{i,d}\, x_d\right)$$

# Building a Network

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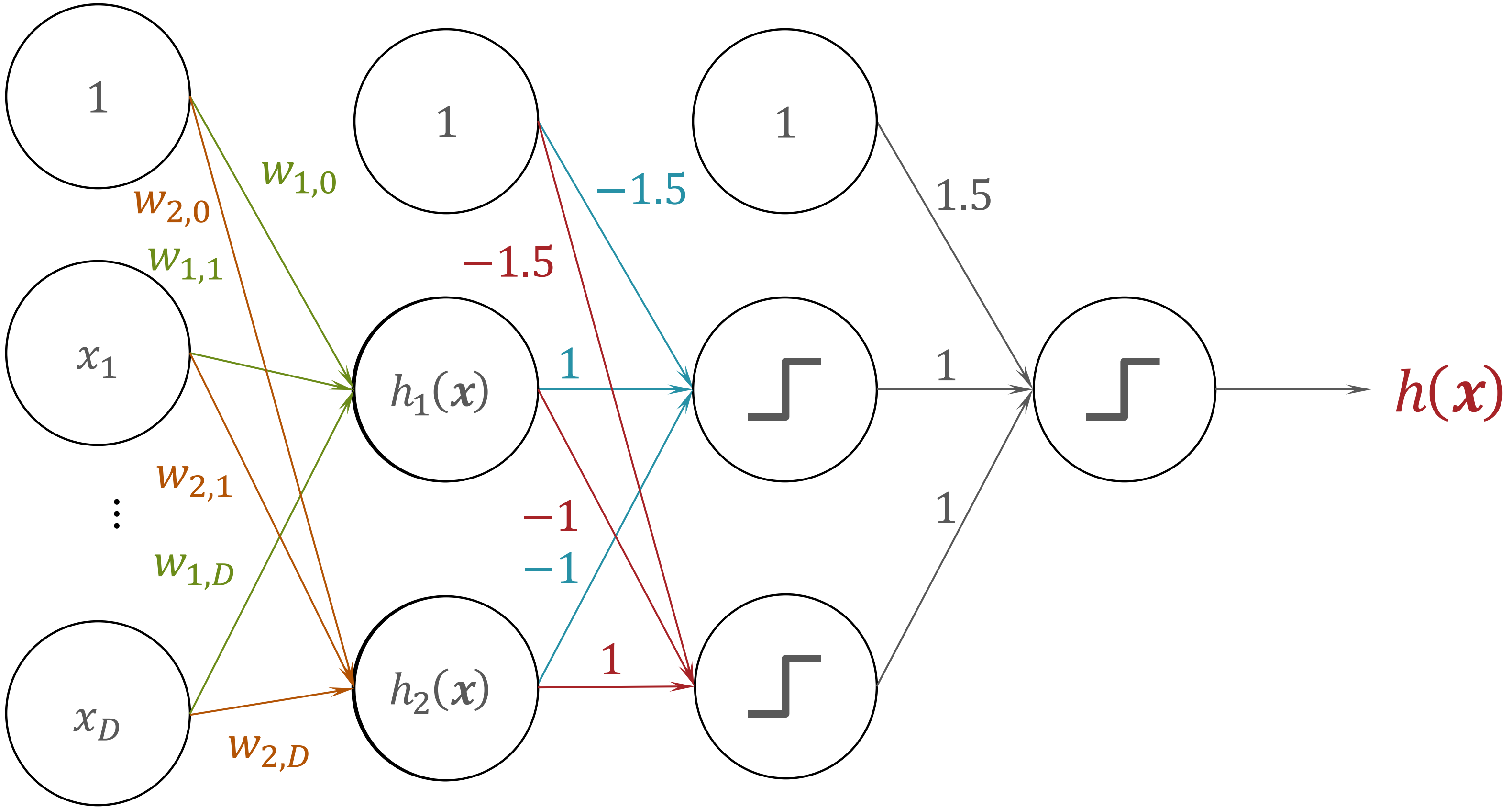


$$h(\boldsymbol{x}) = \text{sign}(\text{sign}(\text{sign}(\boldsymbol{w}_1^T\boldsymbol{x}) - \text{sign}(\boldsymbol{w}_2^T\boldsymbol{x}) - 1.5) + \text{sign}(-\text{sign}(\boldsymbol{w}_1^T\boldsymbol{x}) + \text{sign}(\boldsymbol{w}_2^T\boldsymbol{x}) - 1.5) + 1.5)$$

# Building a Network

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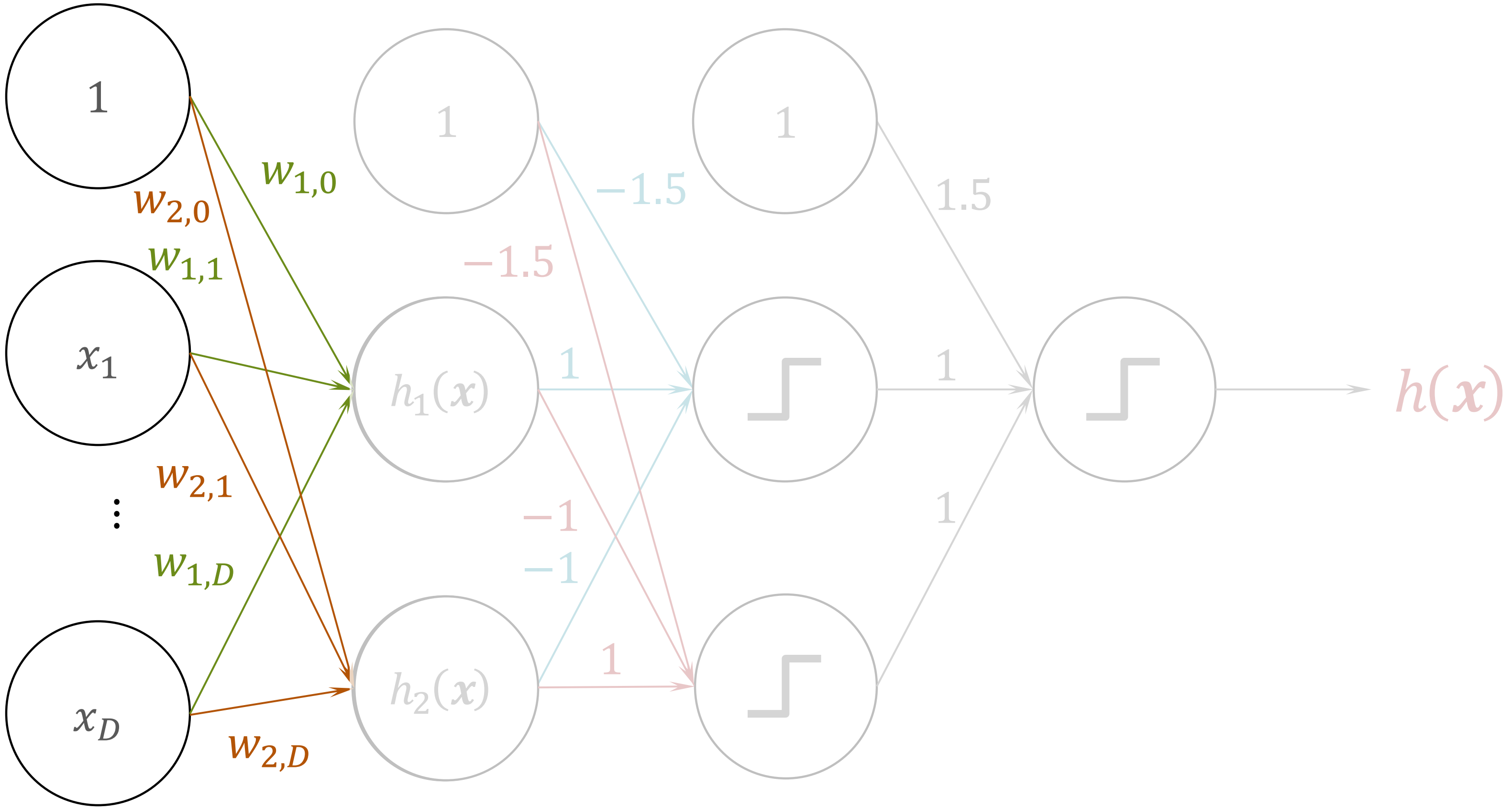


$$h(\boldsymbol{x}) = \text{sign}(\text{sign}(\text{sign}(\boldsymbol{w}_1^T\boldsymbol{x}) - \text{sign}(\boldsymbol{w}_2^T\boldsymbol{x}) - 1.5) + \text{sign}(-\text{sign}(\boldsymbol{w}_1^T\boldsymbol{x}) + \text{sign}(\boldsymbol{w}_2^T\boldsymbol{x}) - 1.5) + 1.5)$$

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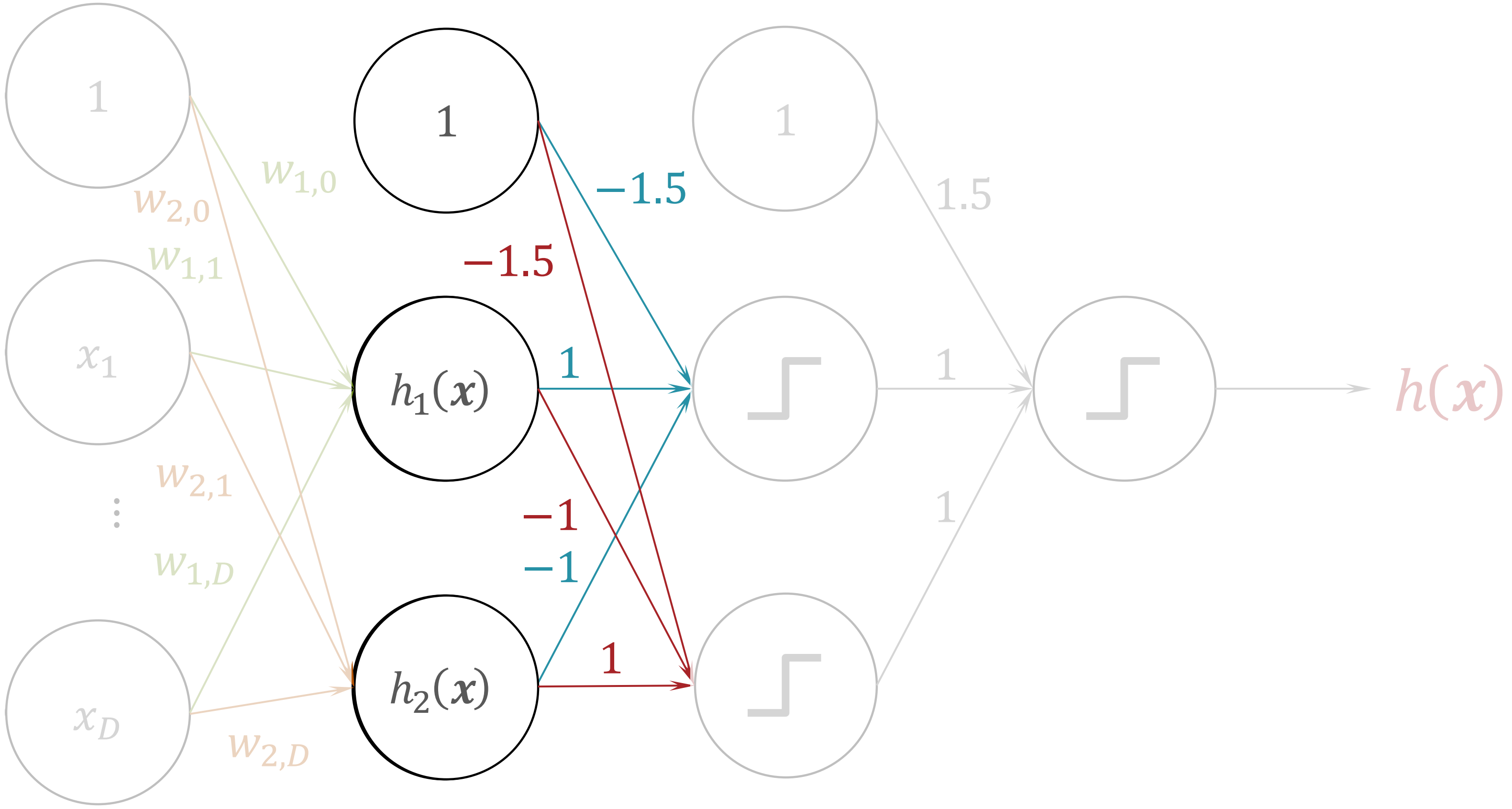


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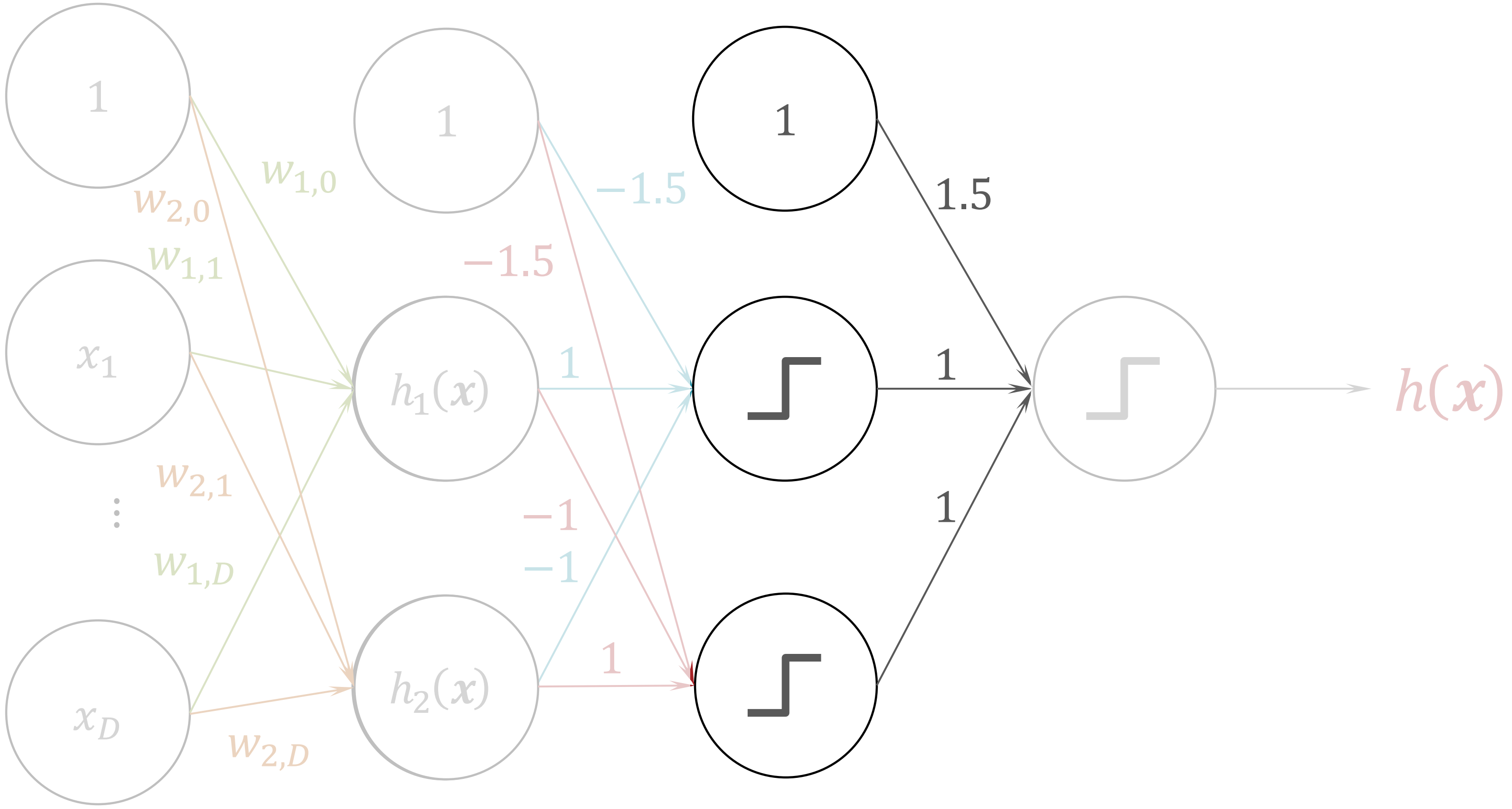


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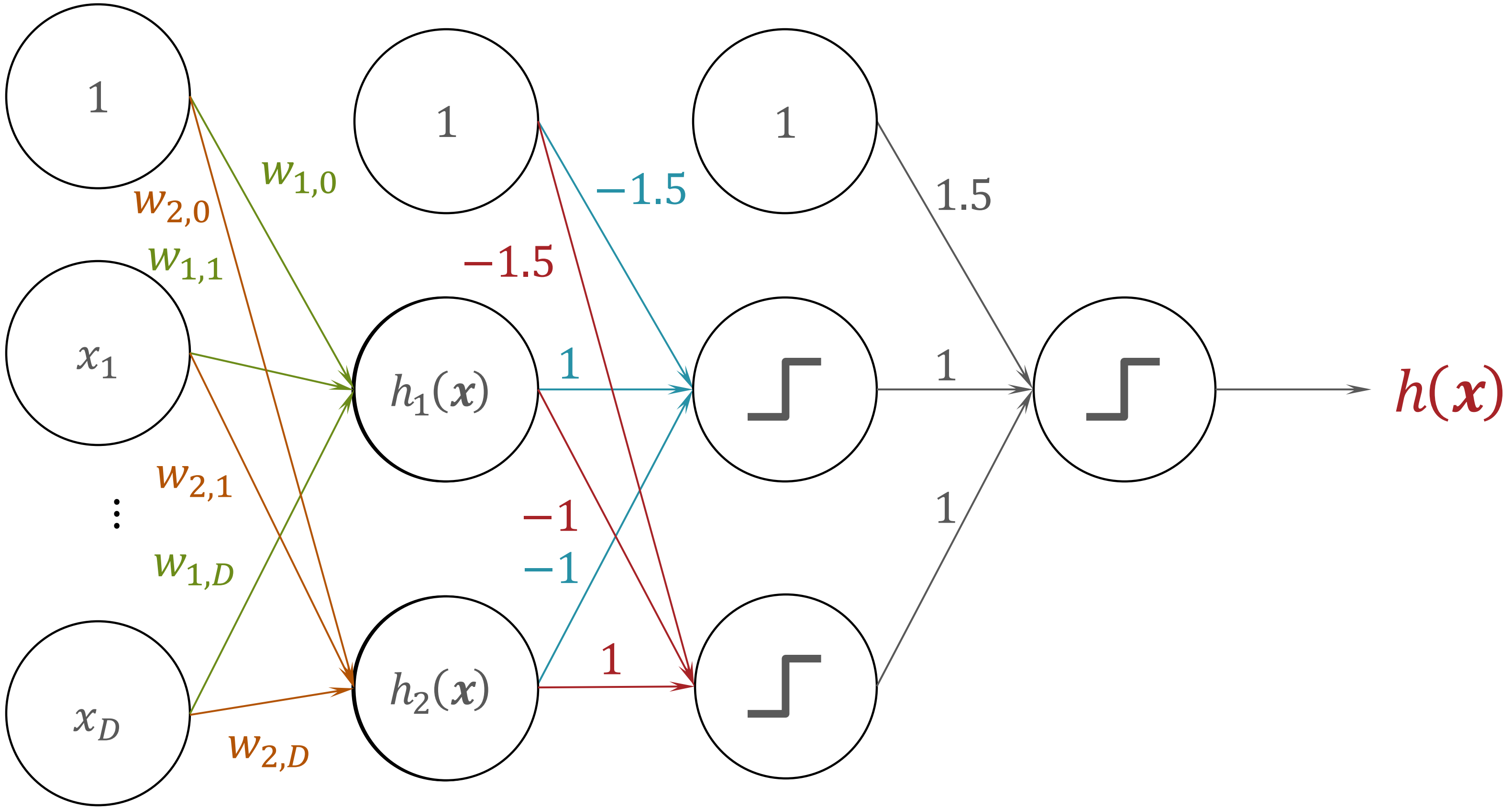


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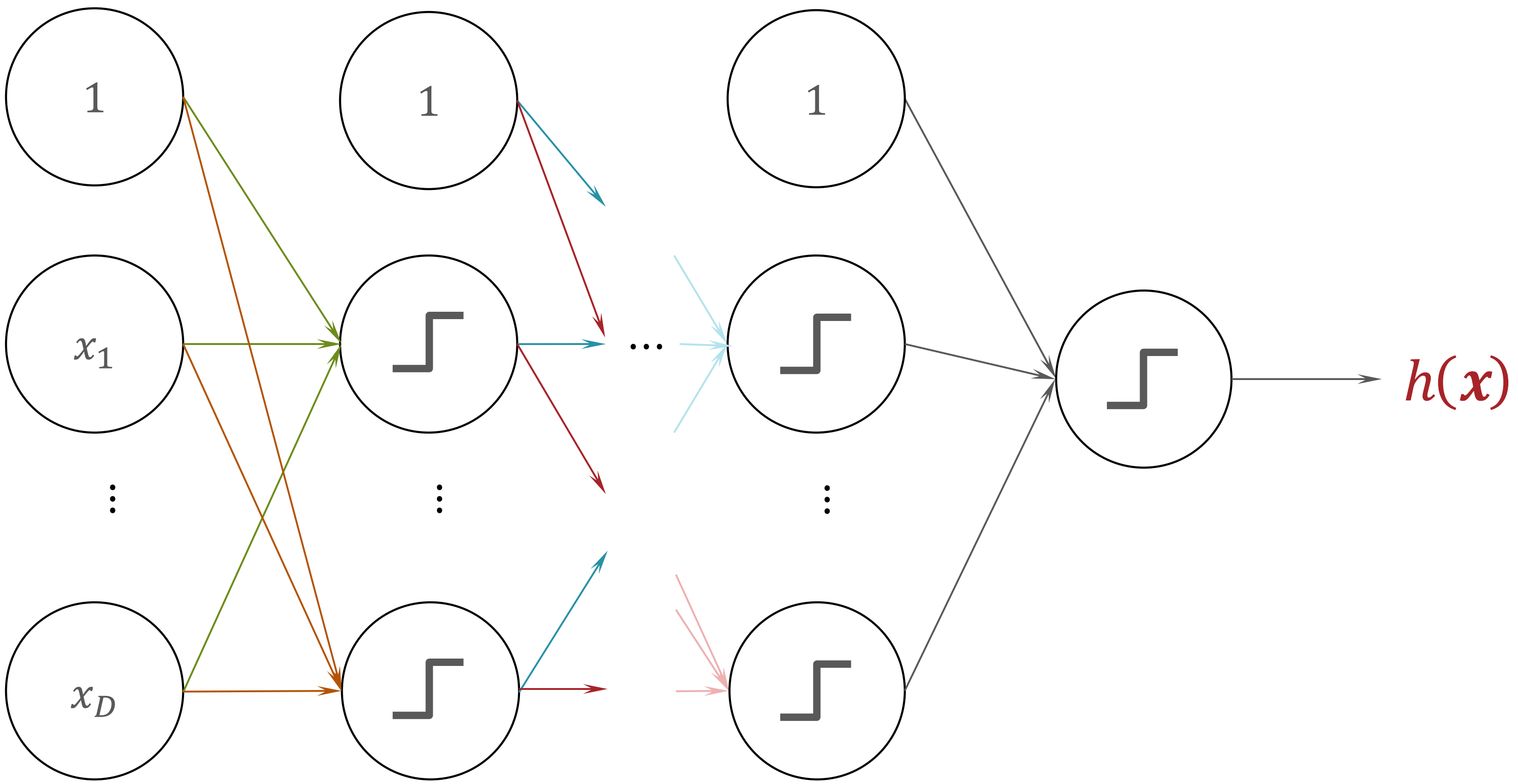
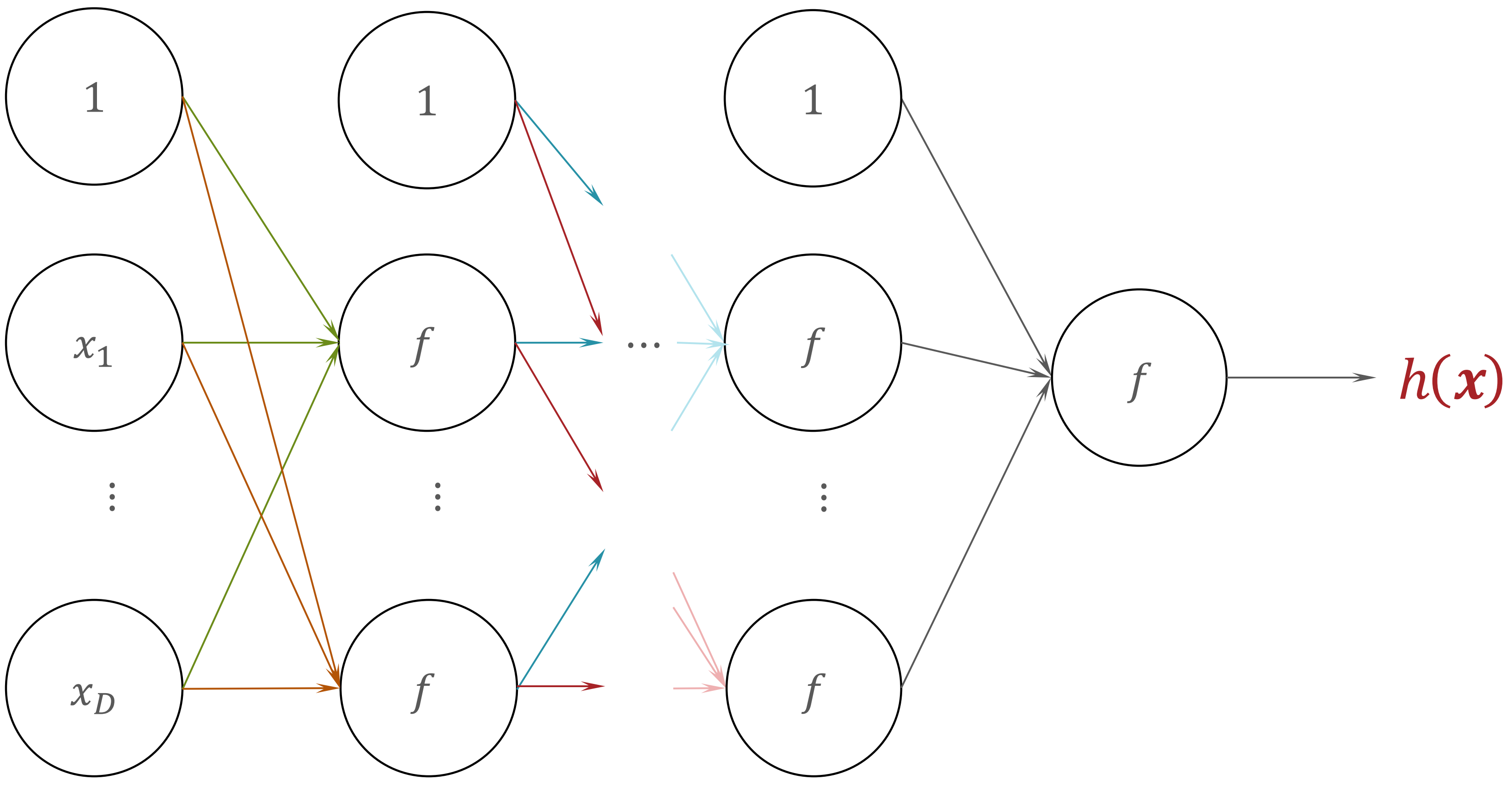
$$\text{sign}(-\text{sign}(\boldsymbol{w}_1^T\boldsymbol{x}) + \text{sign}(\boldsymbol{w}_2^T\boldsymbol{x}) - 1.5) + 1.5)$$

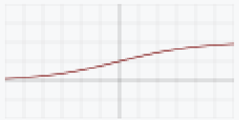
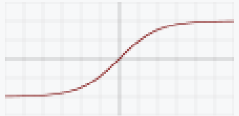
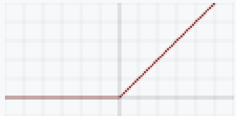
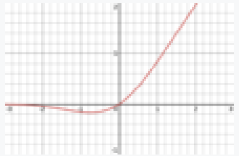
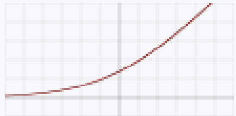
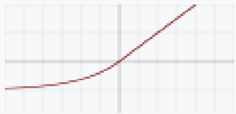
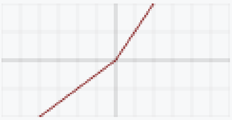
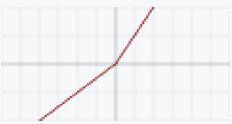
# Multi-Layer Perceptron (MLP)



# (Fully-Connected) Feed Forward Neural Network



# Activation Functions

| | | |
|---|---|---|
| Logistic, sigmoid, or soft step |  | $\sigma(x) = \dfrac{1}{1+e^{-x}}$ |
| Hyperbolic tangent (tanh) |  | $\tanh(x) = \dfrac{e^x - e^{-x}}{e^x + e^{-x}}$ |
| Rectified linear unit (ReLU)[7] |  | $\begin{cases} 0 & \text{if } x \le 0 \\ x & \text{if } x > 0 \end{cases}$ $= \max\{0, x\} = x\mathbf{1}_{x>0}$ |
| Gaussian Error Linear Unit (GELU)[4] |  | $\frac{1}{2}x\left(1 + \operatorname{erf}\left(\frac{x}{\sqrt{2}}\right)\right)$ $= x\Phi(x)$ |
| Softplus[8] |  | $\ln(1+e^x)$ |
| Exponential linear unit (ELU)[9] |  | $\begin{cases} \alpha\left(e^x - 1\right) & \text{if } x \le 0 \\ x & \text{if } x > 0 \end{cases}$ with parameter $\alpha$ |
| Leaky rectified linear unit (Leaky ReLU)[11] |  | $\begin{cases} 0.01x & \text{if } x < 0 \\ x & \text{if } x \ge 0 \end{cases}$ |
| Parametric rectified linear unit (PReLU)[12] |  | $\begin{cases} \alpha x & \text{if } x < 0 \\ x & \text{if } x \ge 0 \end{cases}$ with parameter $\alpha$ |

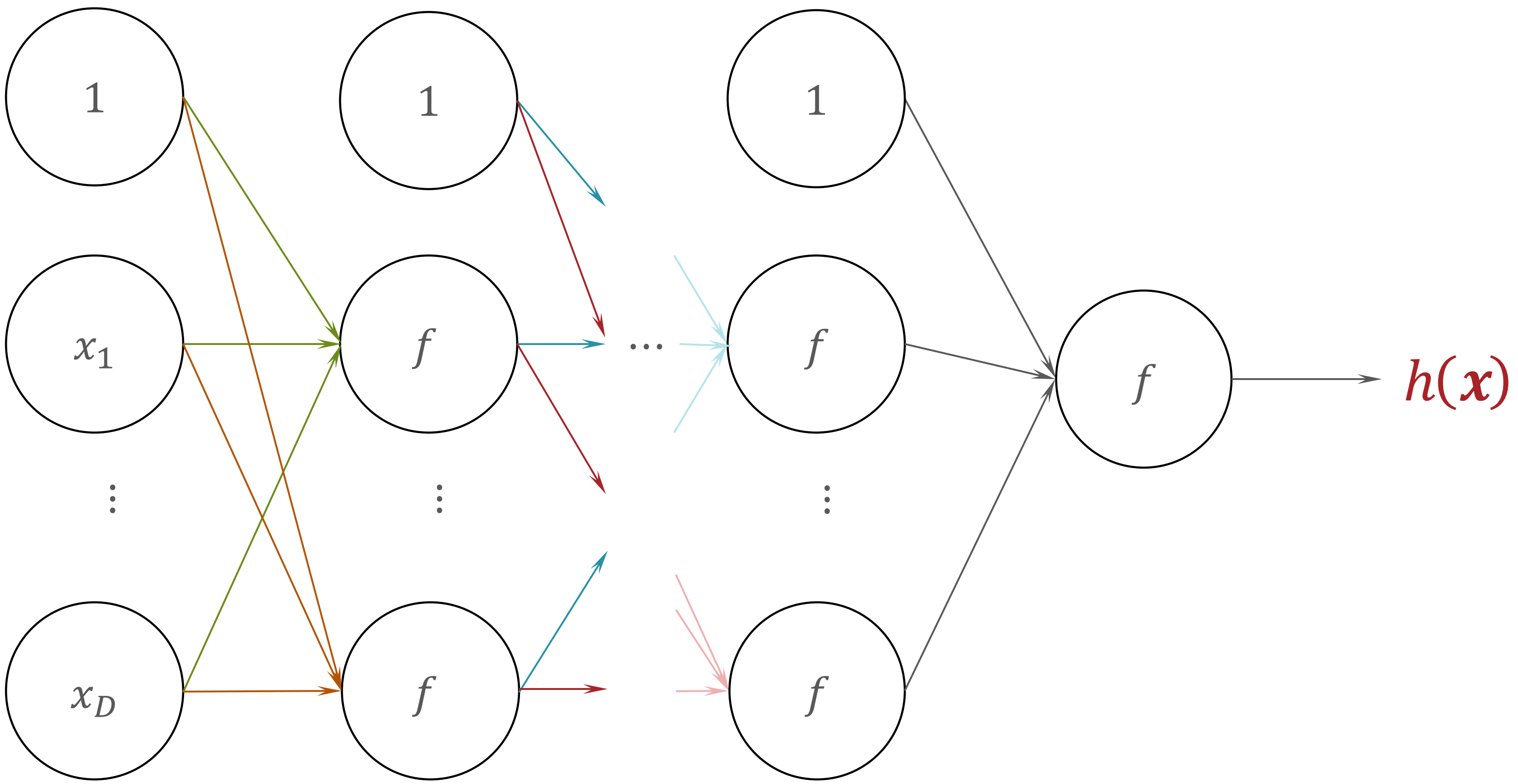


Source: https://en.wikipedia.org/wiki/Activation_function

## Poll Question 1

True or False: Linear and logistic regression models can be expressed as neural networks.

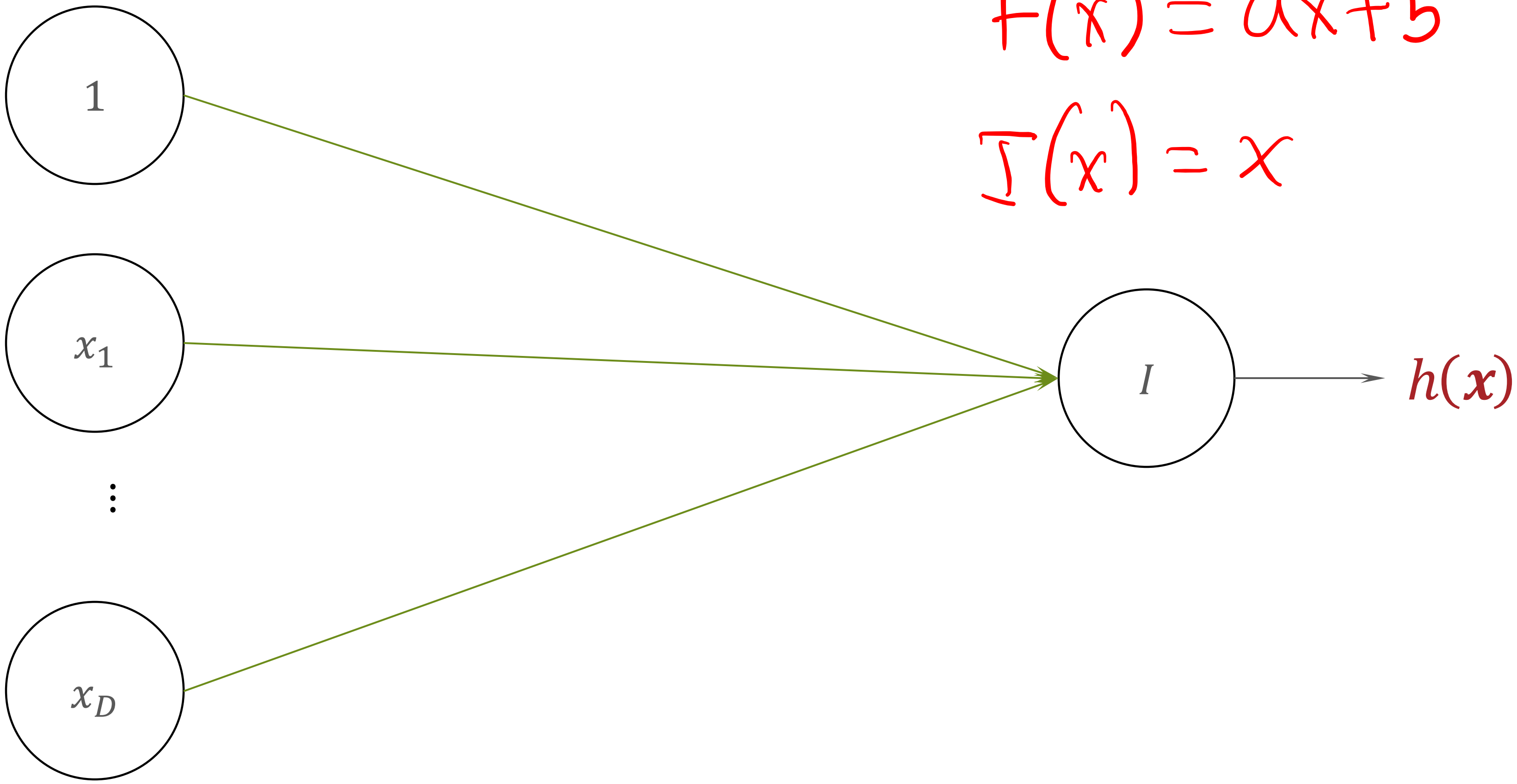
A. Only true for linear regression
B. Only true for logistic regression
C. TOXIC
D. True for both
E. False for both



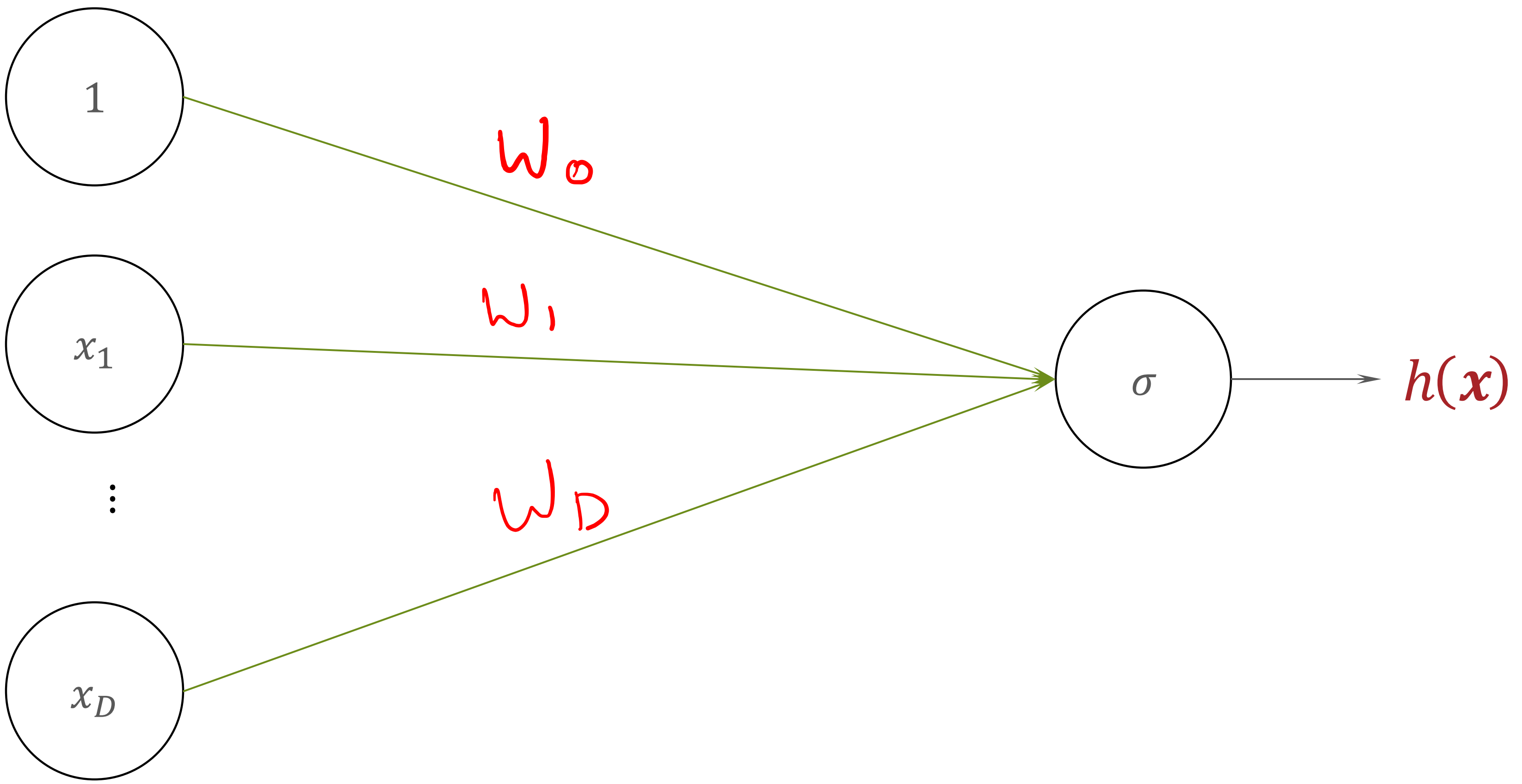
# Linear Regression as a Neural Network

$f(x) = ax + b$

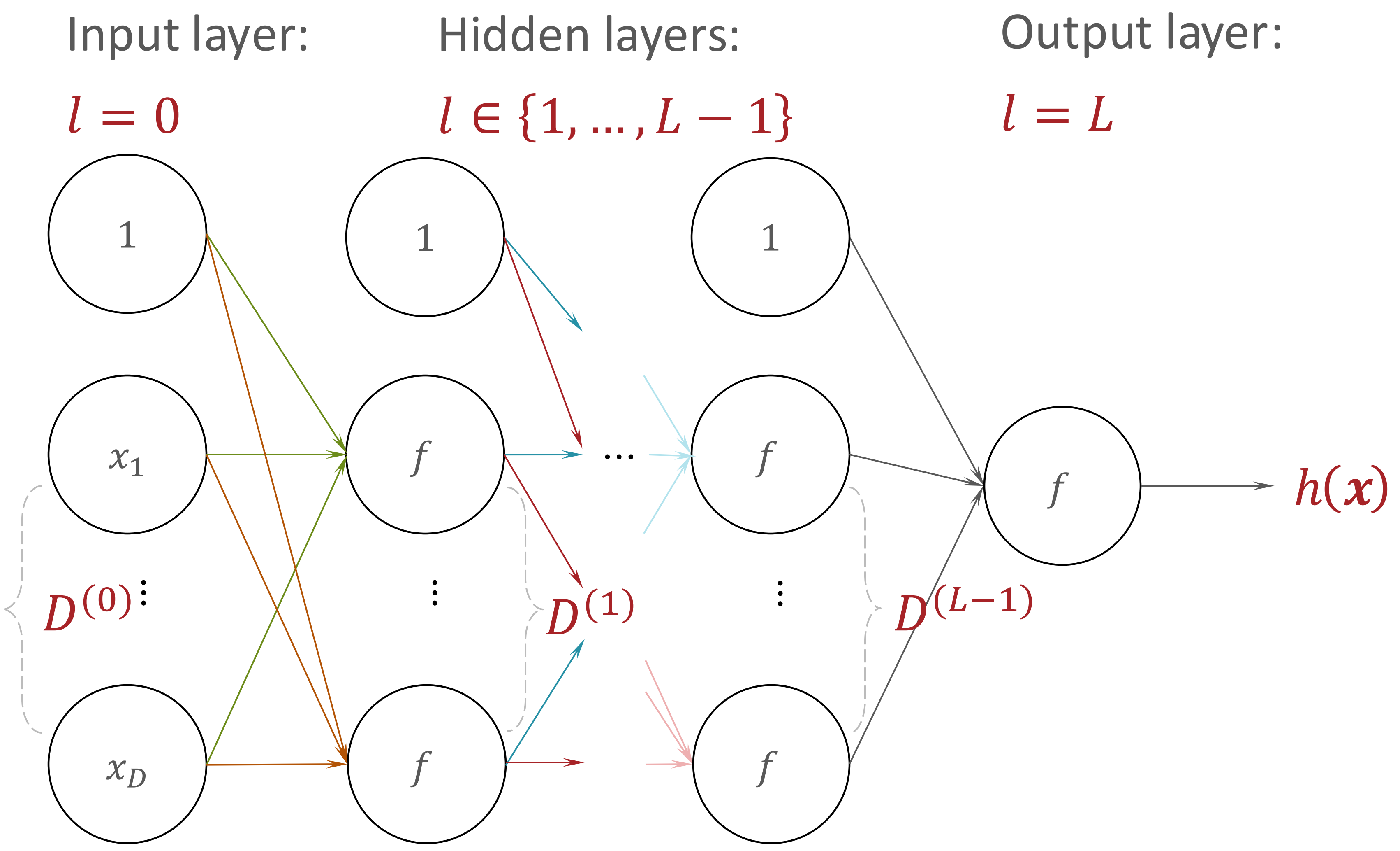
$I(x) = x$



# Logistic Regression as a Neural Network



# (Fully-Connected) Feed Forward Neural Network

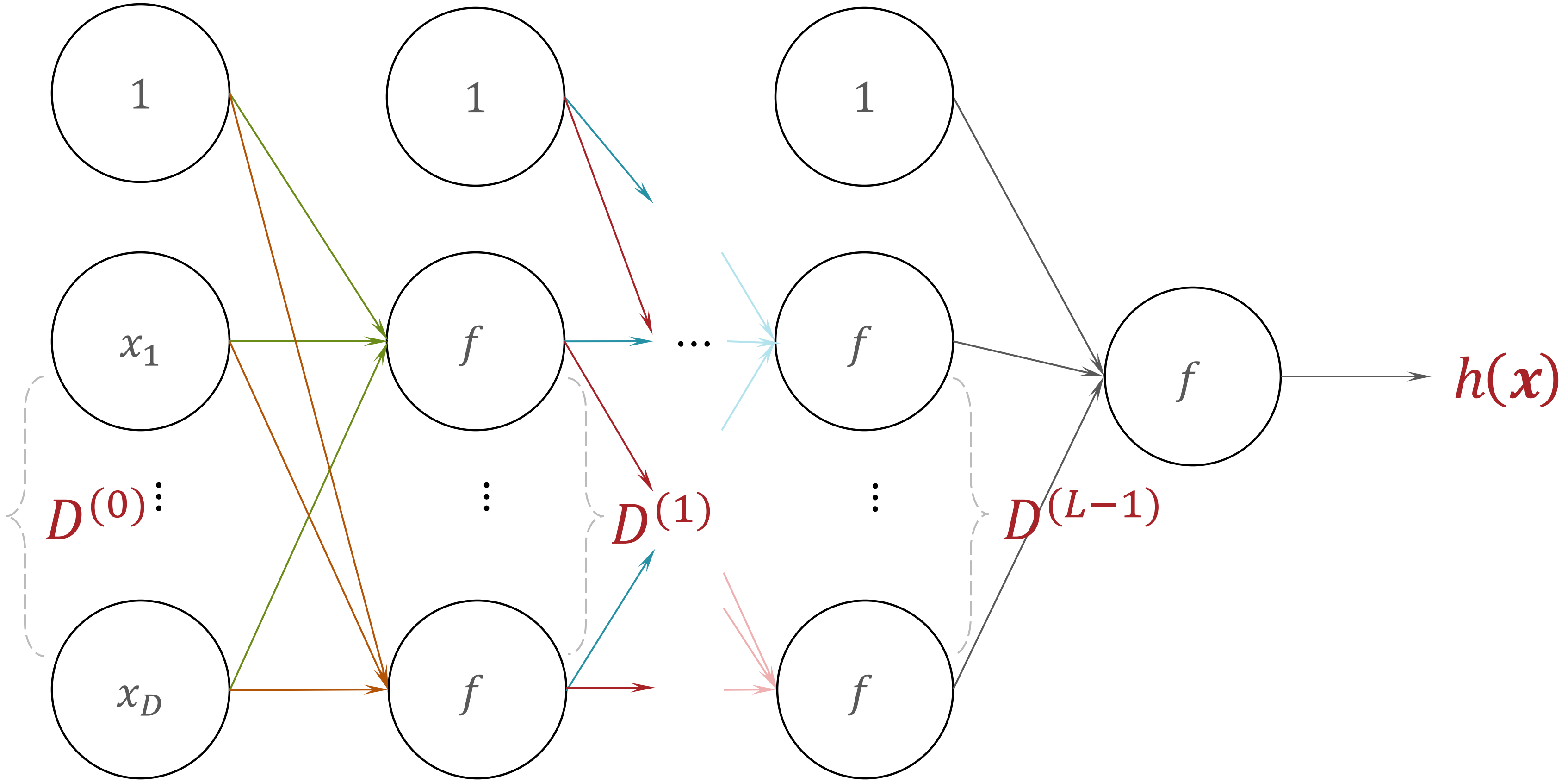



Layer $l$ has dimension $D^{(l)}$ → Layer $l$ has $D^{(l)} + 1$ nodes, counting the bias node

# (Fully-Connected) Feed Forward Neural Network

The weights between layer $l-1$ and layer $l$ are a matrix:

$W^{(l)} \in \mathbb{R}^{D^{(l)} \times \left(D^{(l-1)}+1\right)}$




$w_{j,i}^{(l)}$ is the weight between node $i$ in layer $l-1$ and node $j$ in layer $l$

# So what are all these layers doing for us anyway?

The weights between layer $l-1$ and layer $l$ are a matrix:

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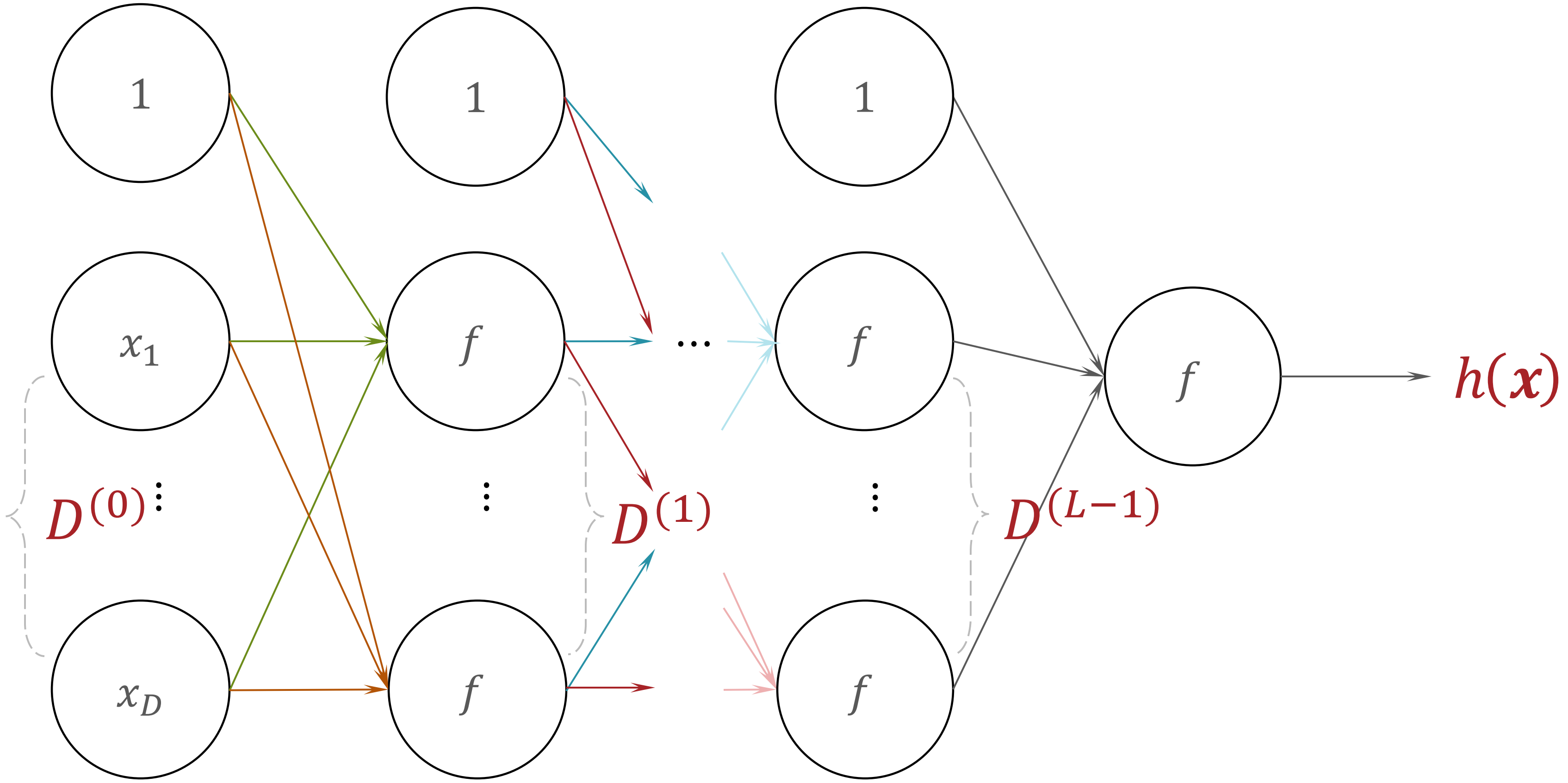


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# Neural Network Decision Boundaries: Example 1

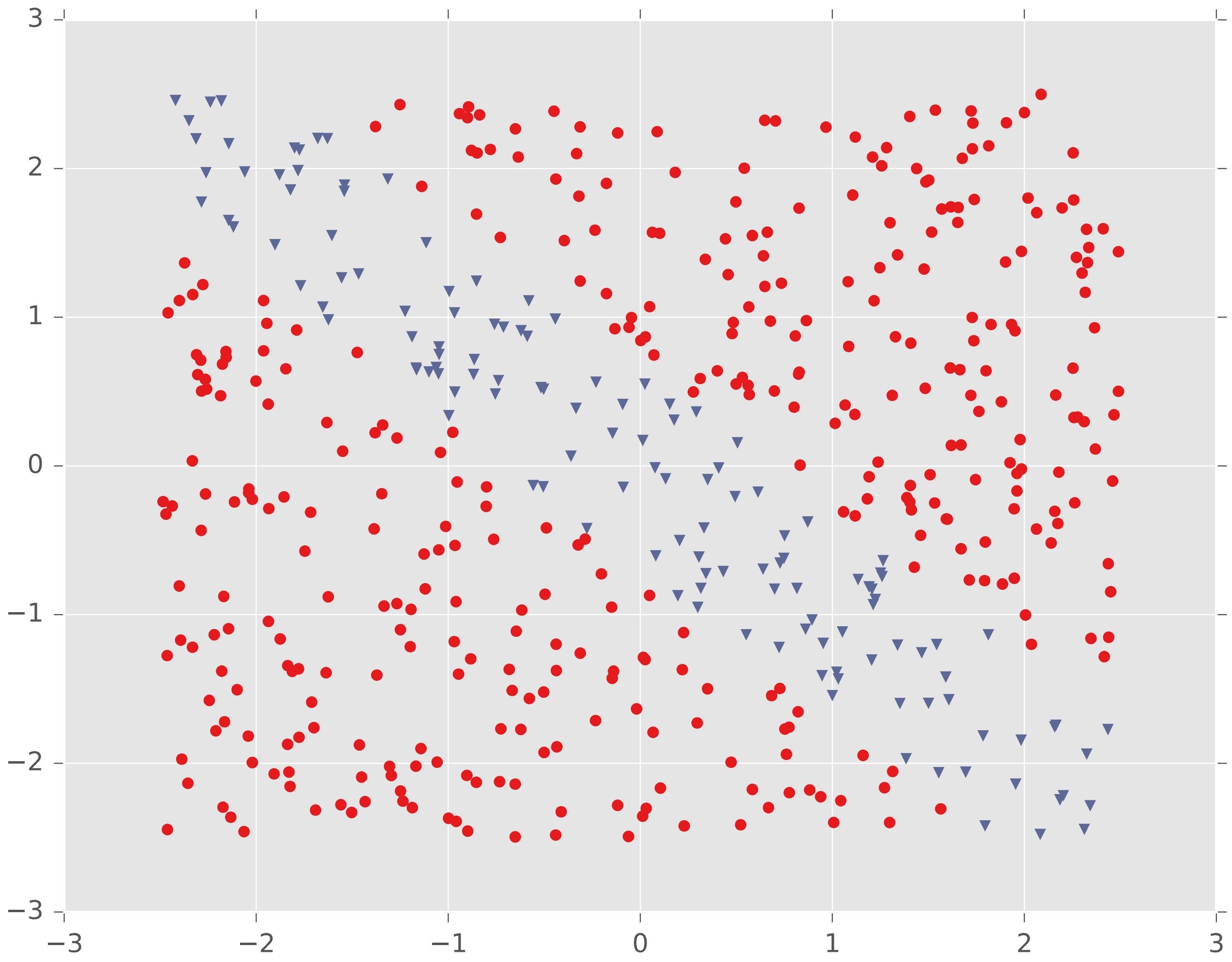


Figure courtesy of Matt Gormley

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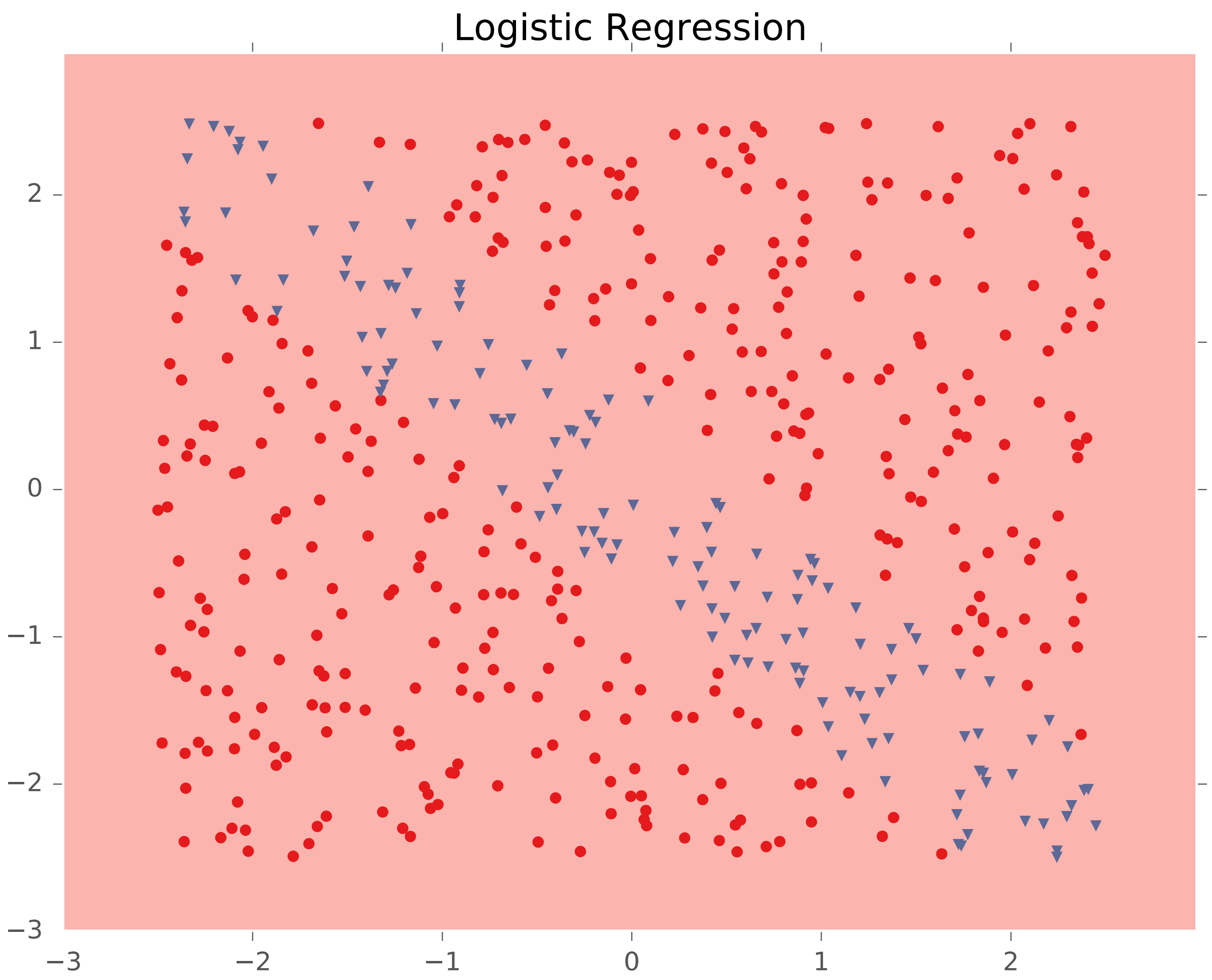


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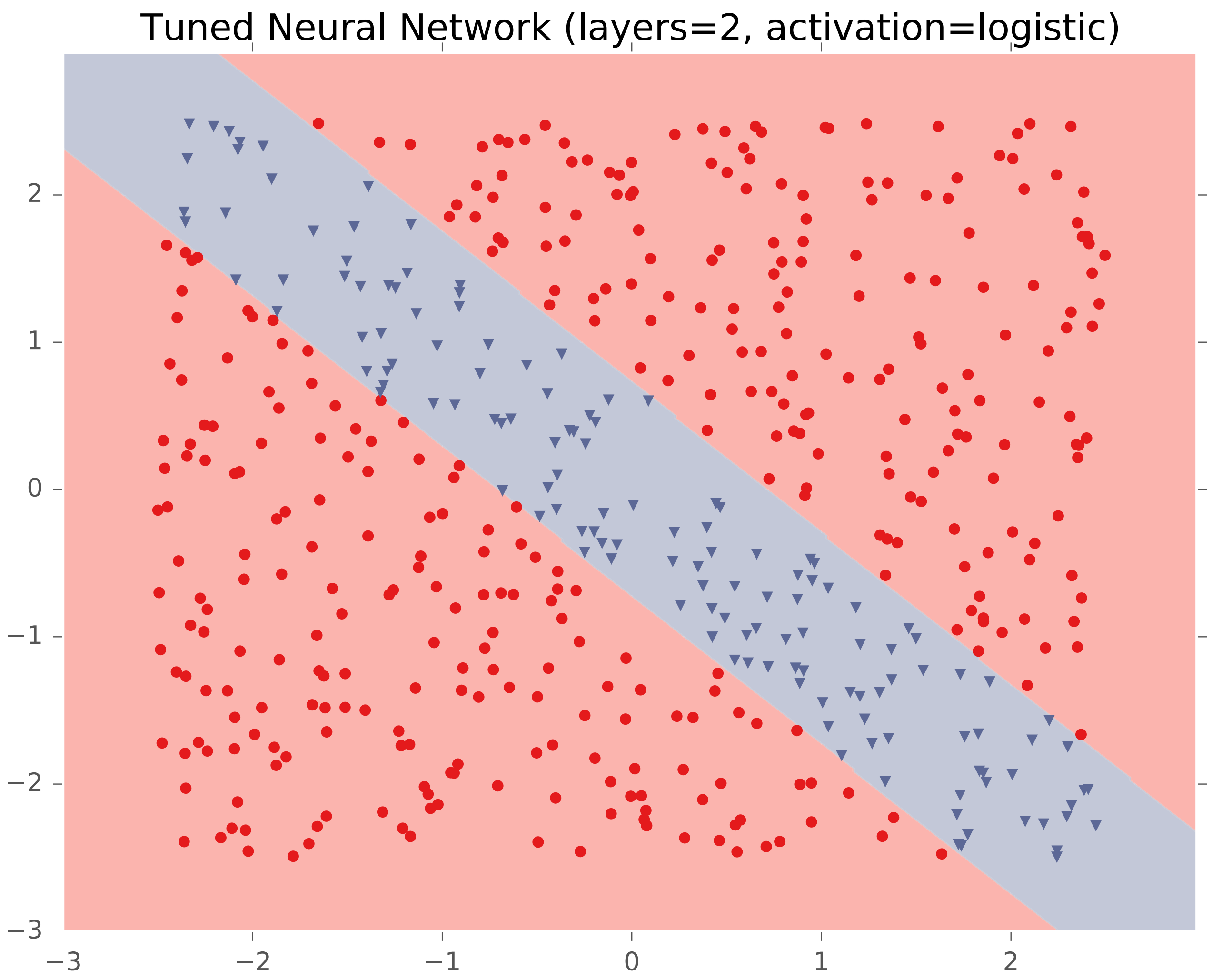


Figure courtesy of Matt Gormley

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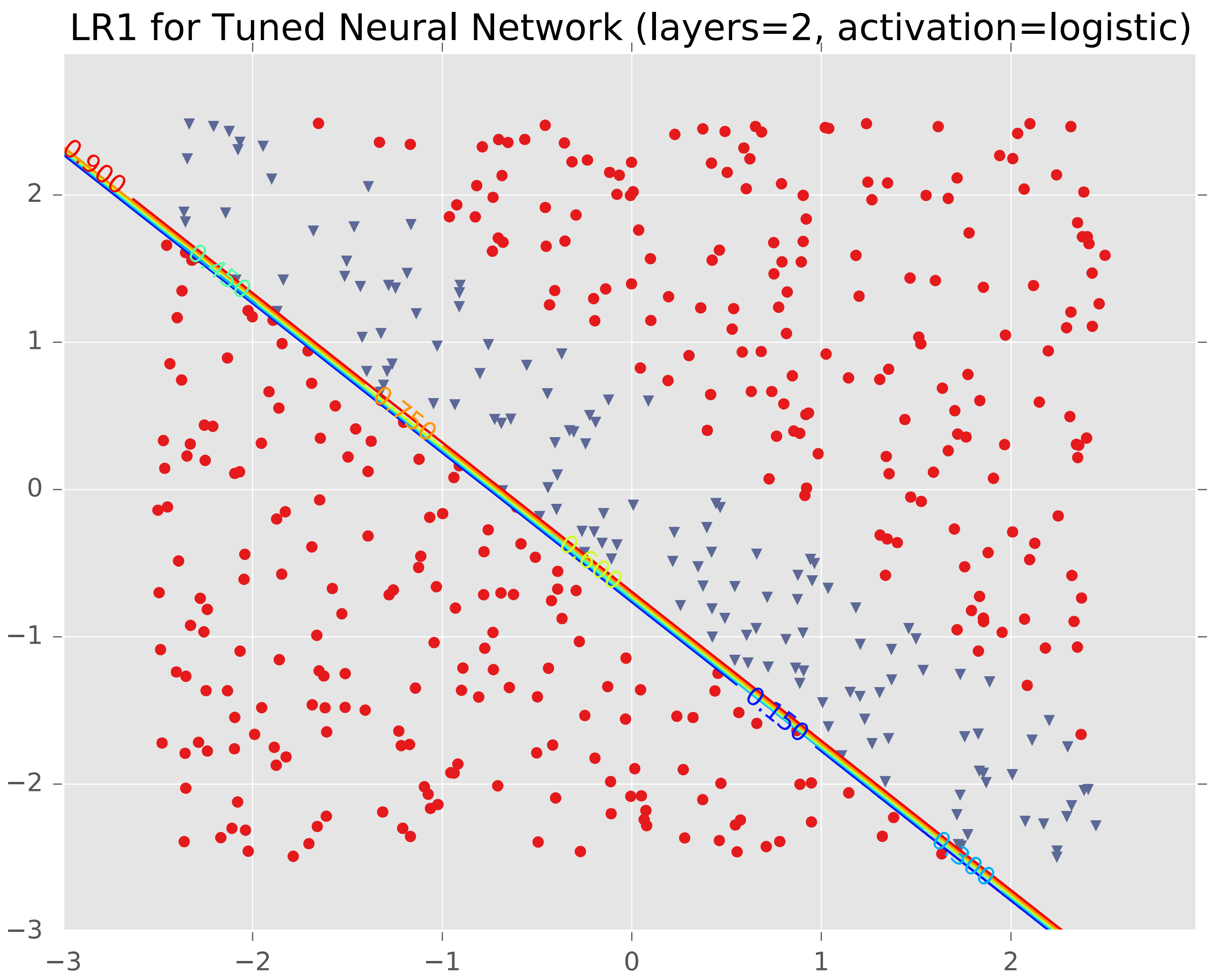


Figure courtesy of Matt Gormley

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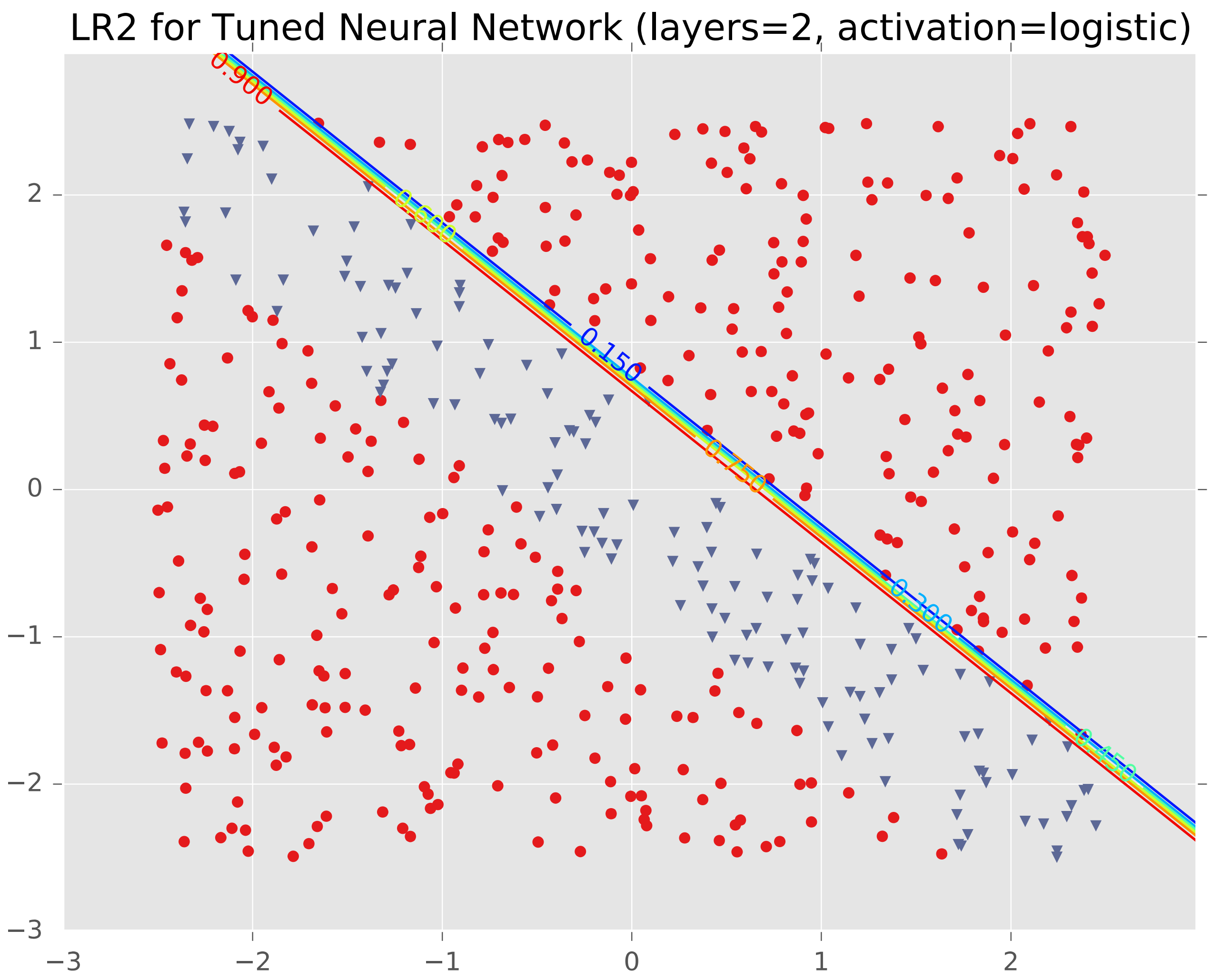


Figure courtesy of Matt Gormley

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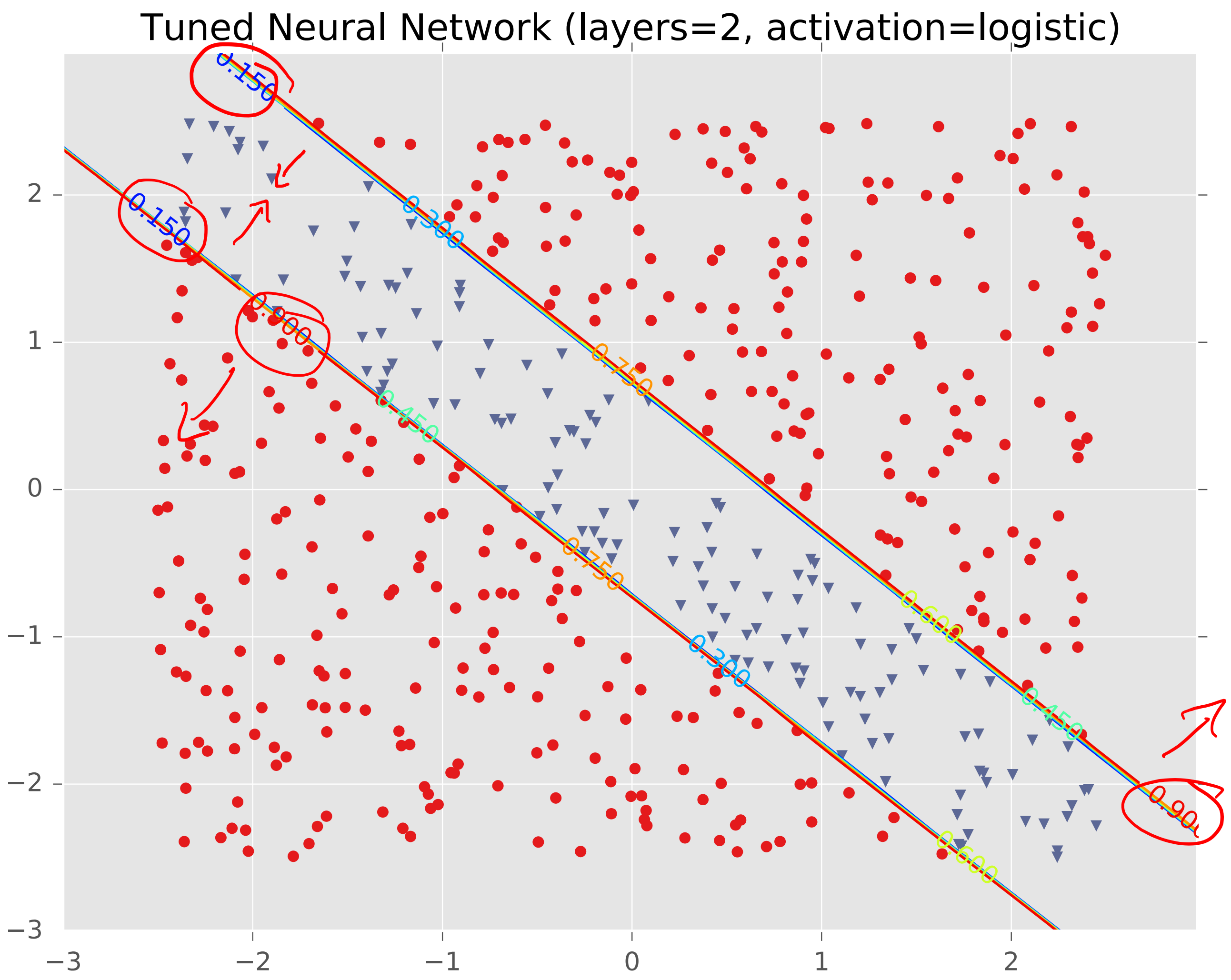


Figure courtesy of Matt Gormley

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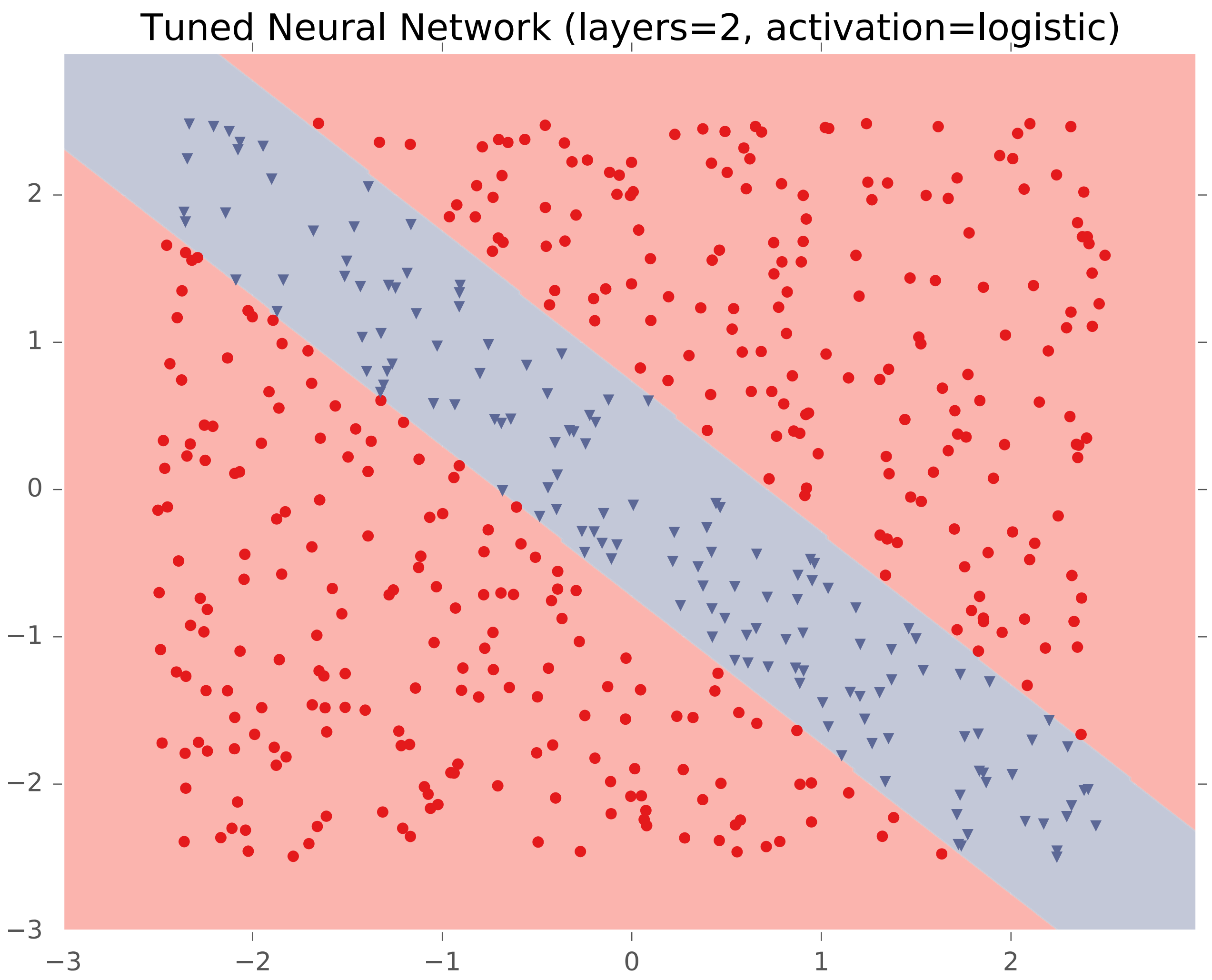


Figure courtesy of Matt Gormley

# Neural Network Decision Boundaries: Example 2

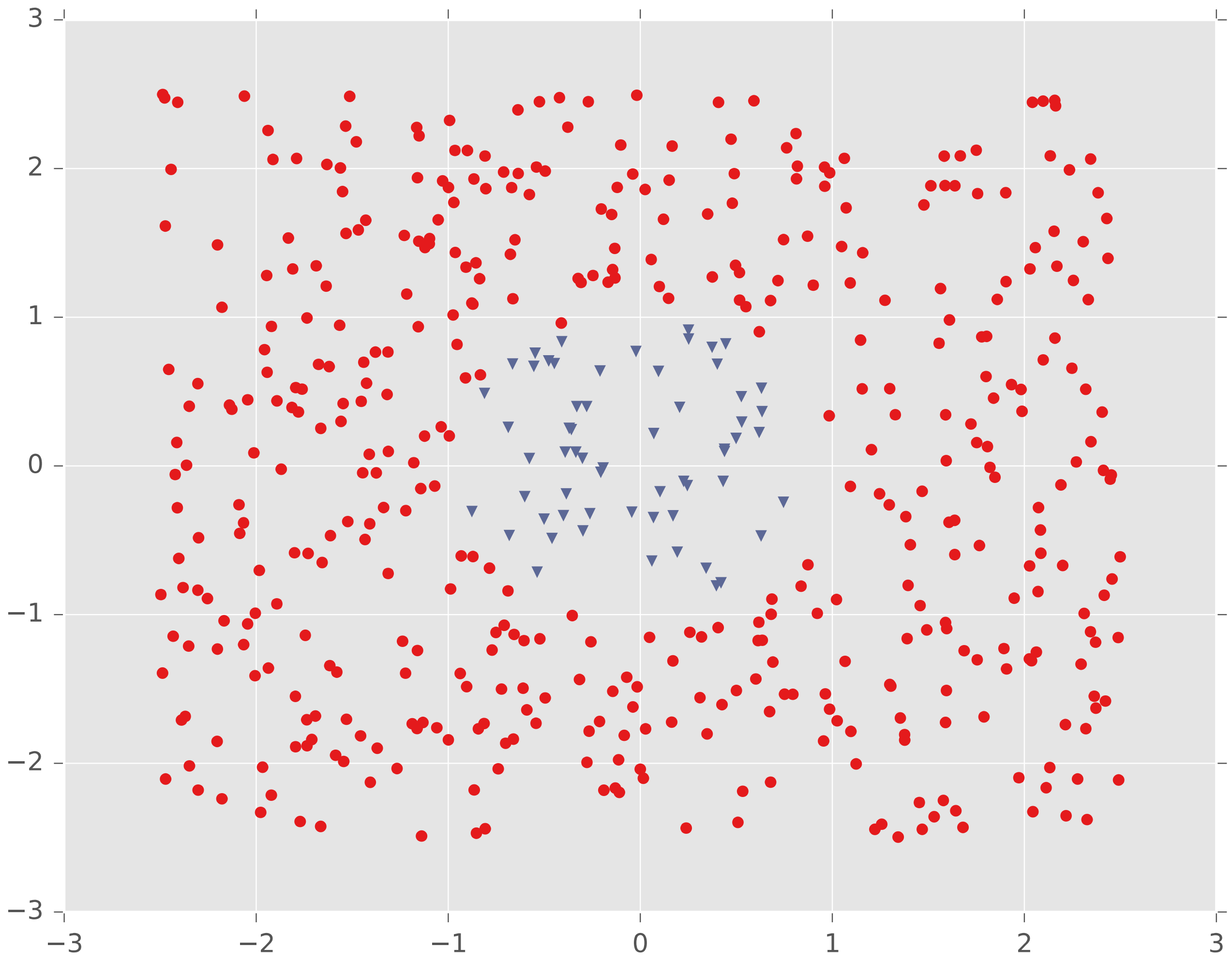


Figure courtesy of Matt Gormley

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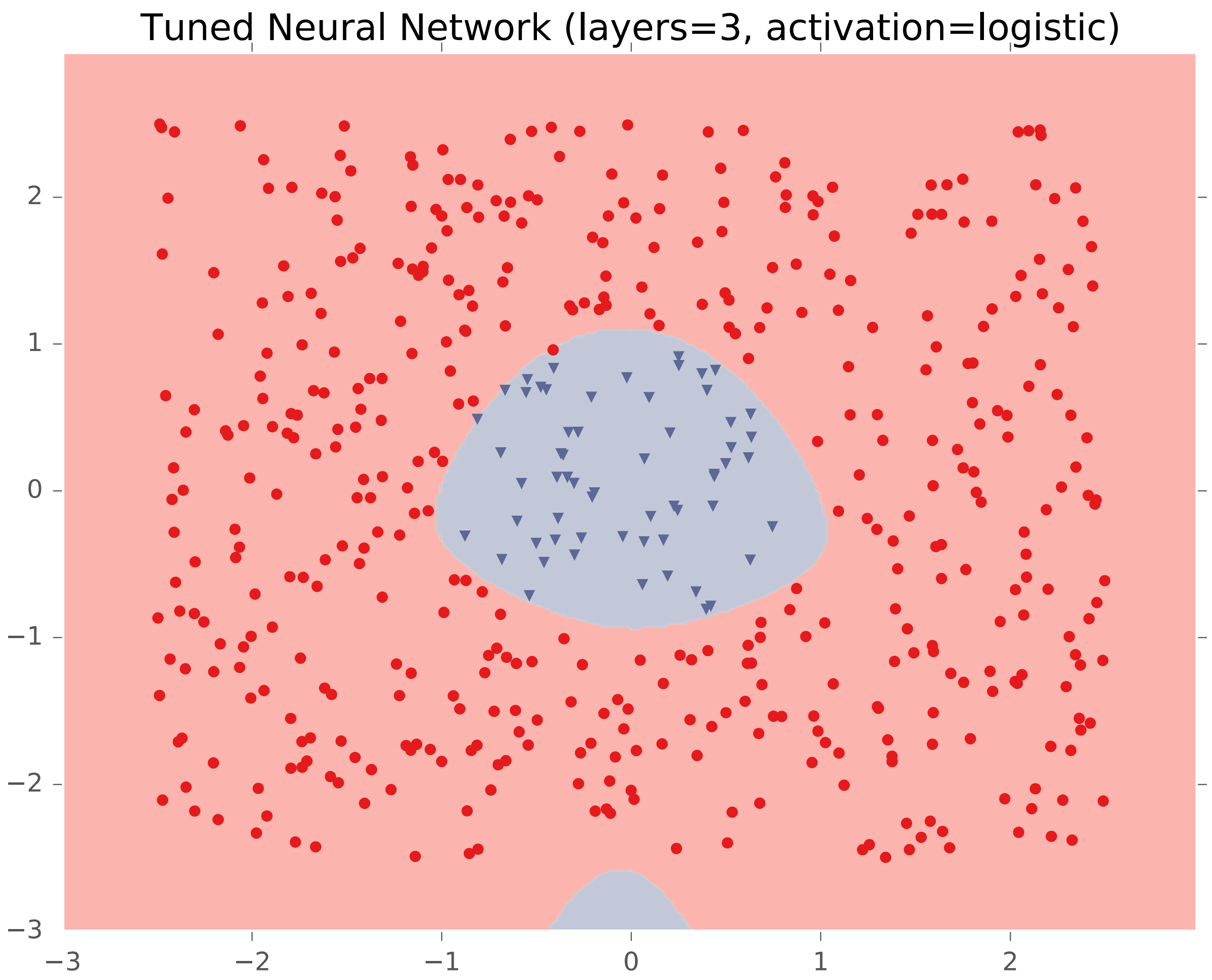




Figure courtesy of Matt Gormley

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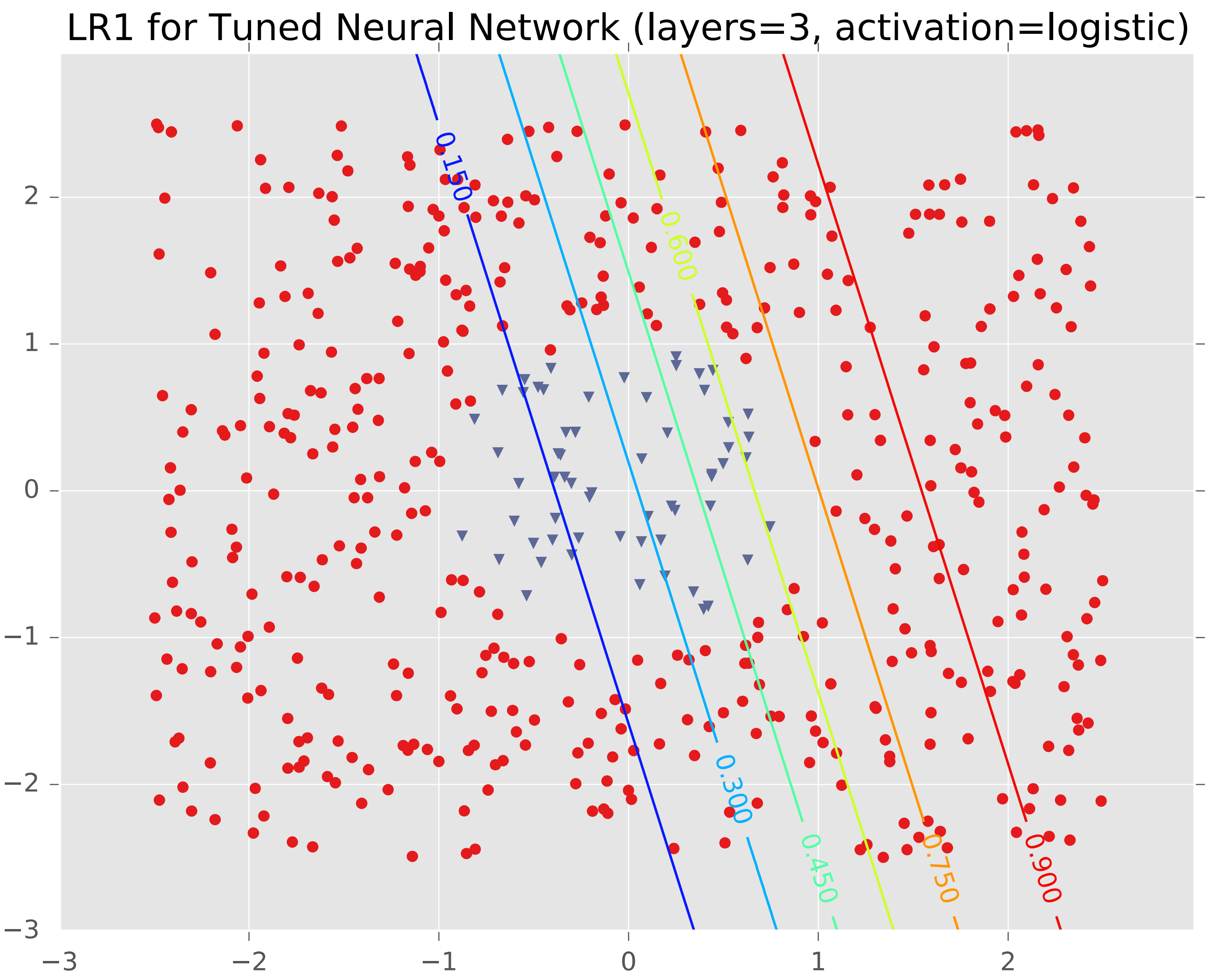


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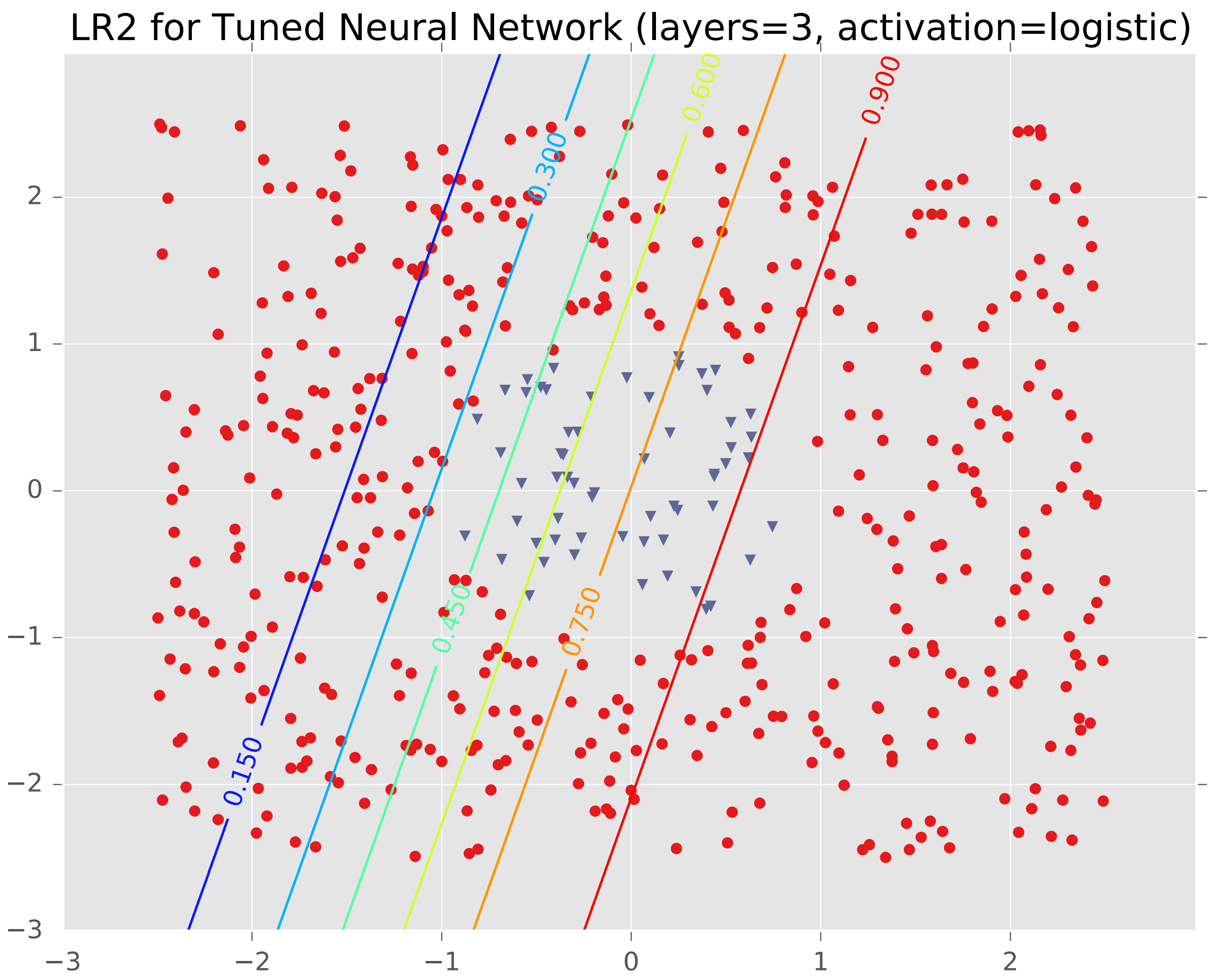


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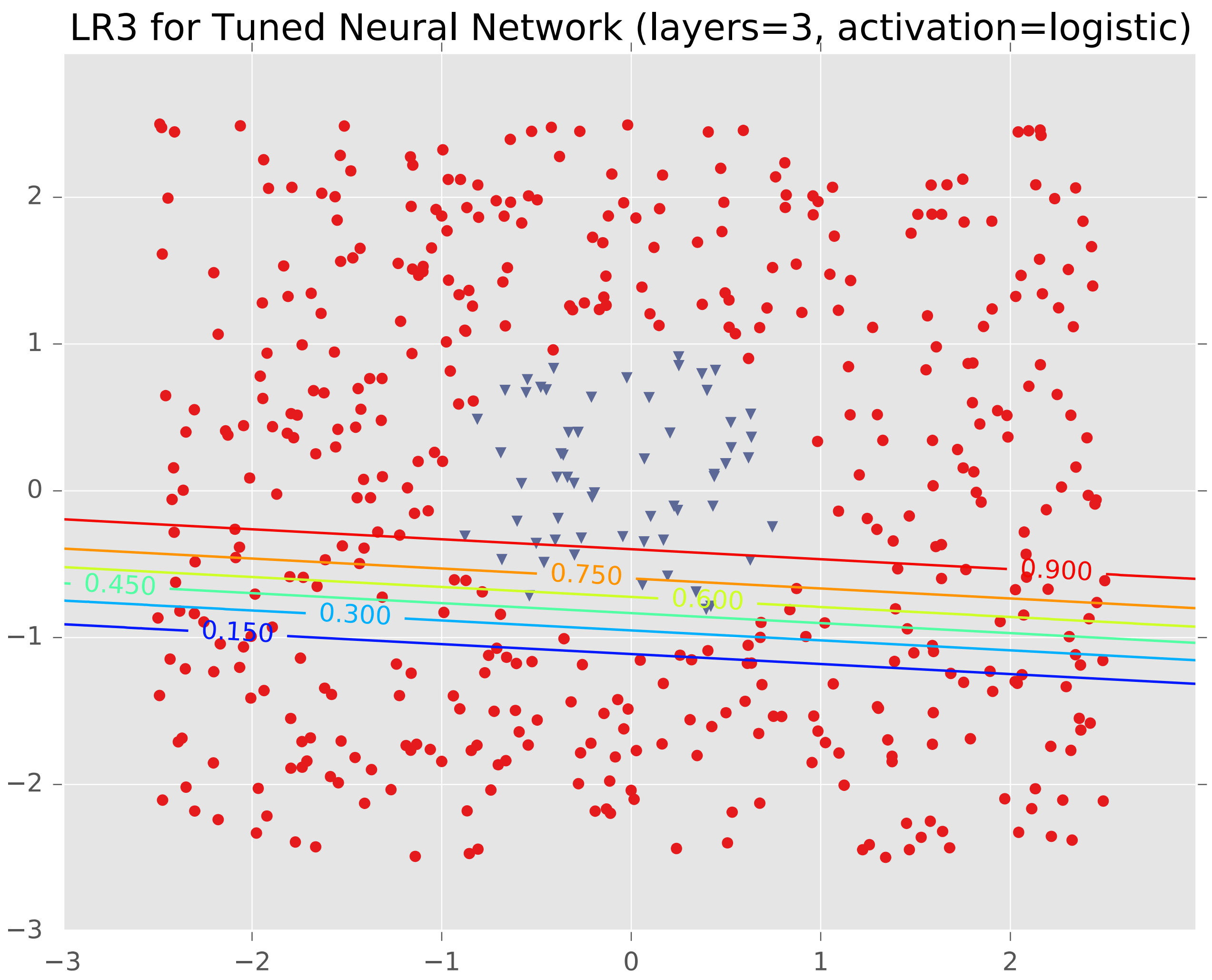


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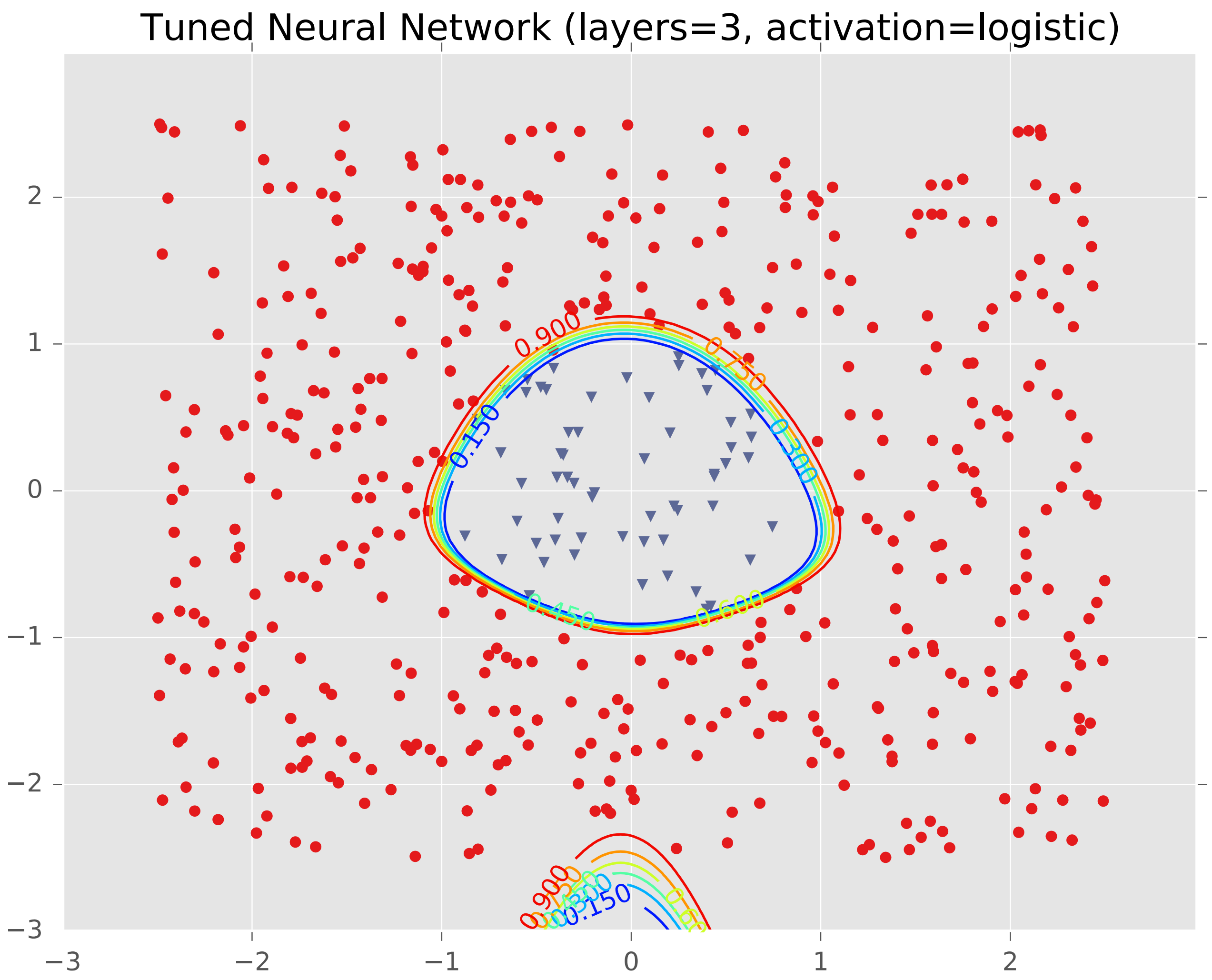



Figure courtesy of Matt Gormley

# Neural Network Decision Boundaries: Example 2

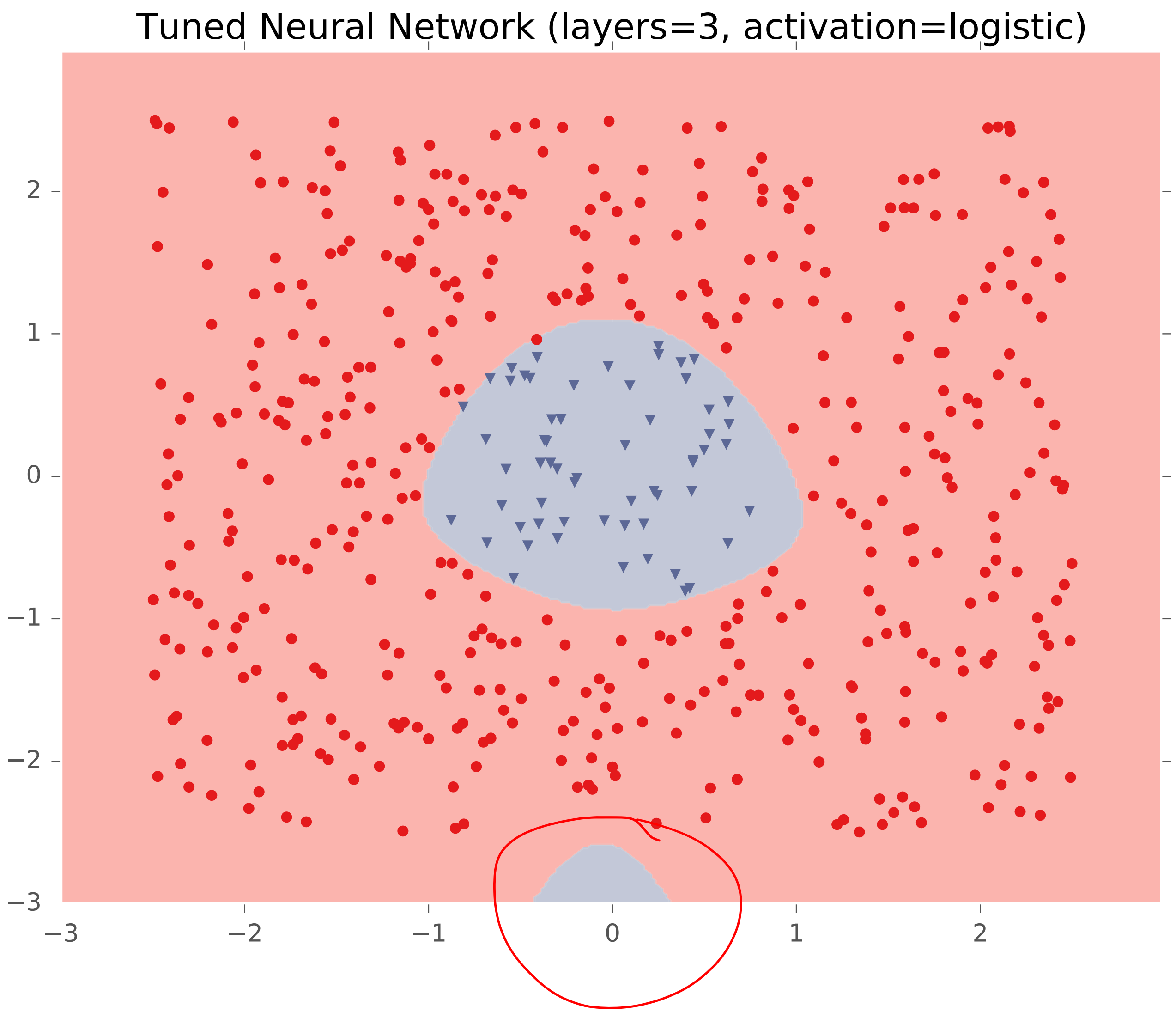
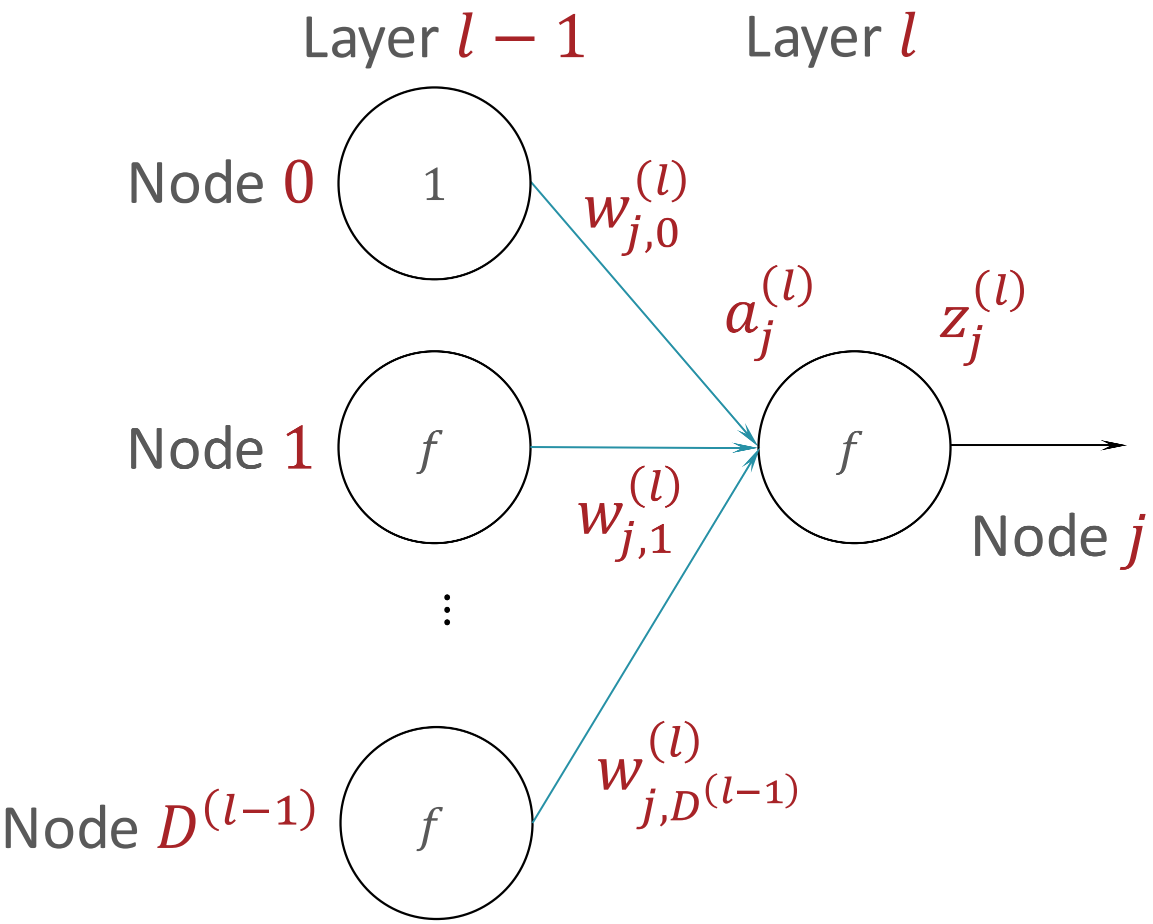



Figure courtesy of Matt Gormley

# Signal and Outputs

Every node has an incoming *signal* and outgoing *output*




$$a_j^{(l)} = \sum_{i=0}^{D^{(l-1)}} w_{j,i}^{(l)} z_i^{(l-1)} \text{ and } z_j^{(l)} = f\left(a_j^{(l)}\right)$$

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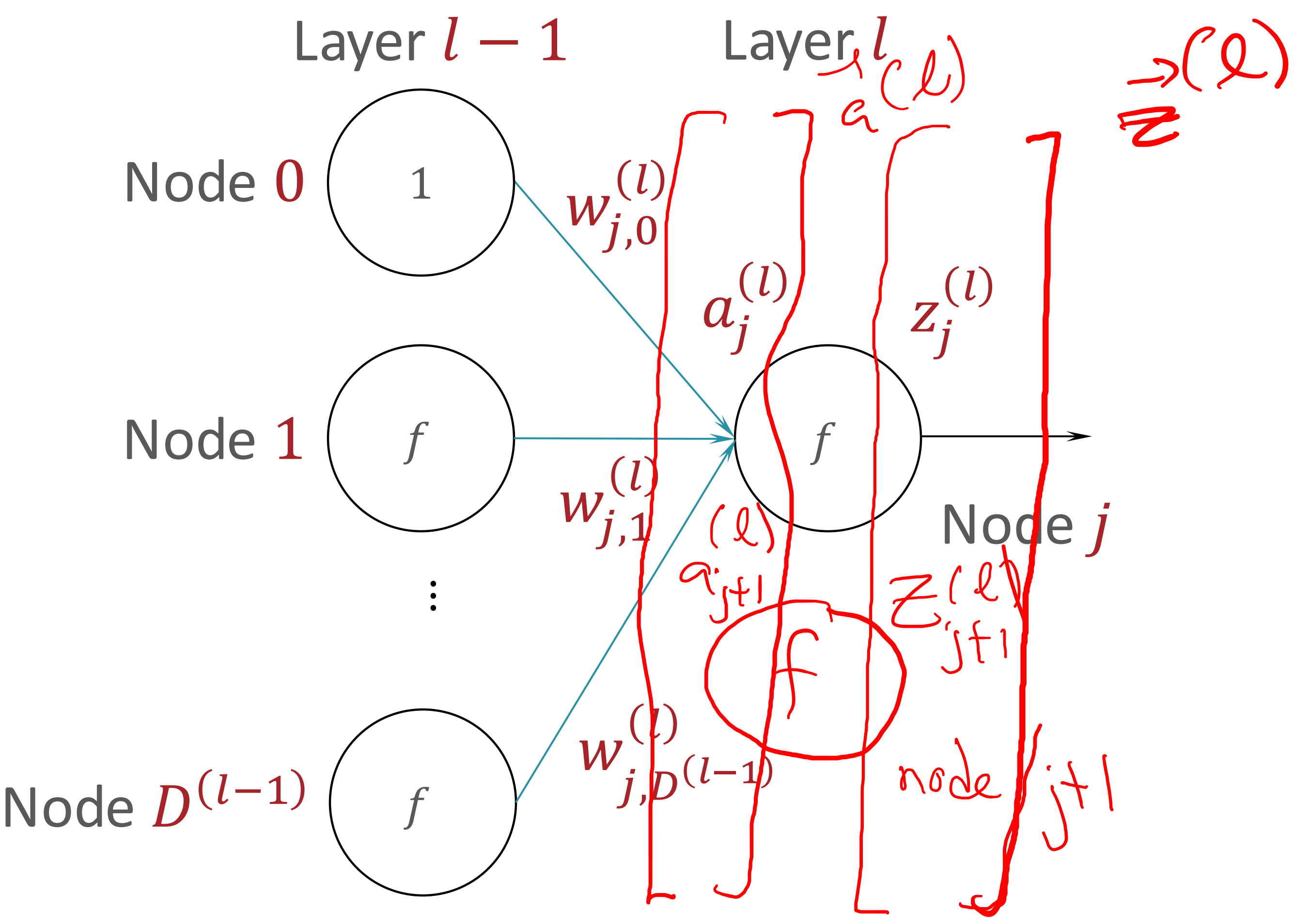



$\boldsymbol{a}^{(l)} = W^{(l)}\underline{\boldsymbol{z}^{(l-1)}}$ and $\boldsymbol{z}^{(l)} = [1, f(\boldsymbol{a}^{(l)})]^T$

# Forward Propagation for Making Predictions

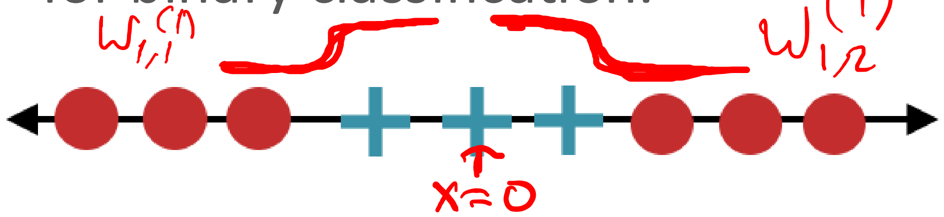
- Input: weights $W^{(1)}, \ldots, W^{(L)}$ and a query data point $\boldsymbol{x}$
- Initialize $\boldsymbol{z}^{(0)} = [1, \boldsymbol{x}]^T$
- For $l = 1, \ldots, L$
  - $\boldsymbol{a}^{(l)} = W^{(l)} \boldsymbol{z}^{(l-1)}$
  - $\boldsymbol{z}^{(l)} = \left[1, f\left(\boldsymbol{a}^{(l)}\right)\right]^T$
- Output: $h_{W^{(1)}, \ldots, W^{(L)}}(\boldsymbol{x}) = \boldsymbol{z}^{(L)}$

# Gradient Descent for Learning

- Input: $\mathcal{D} = \{(\boldsymbol{x}^{(n)}, y^{(n)})\}_{n=1}^{N}, \eta^{(0)}$
- Initialize all weights $W_{(0)}^{(1)}, \dots, W_{(0)}^{(L)}$ to small, random numbers and set $t = 0$
- While TERMINATION CRITERION is not satisfied
  - For $l = 1, \dots, L$
    - Compute $G^{(l)} = \nabla_{W^{(l)}} \ell_{\mathcal{D}}\left(W_{(t)}^{(1)}, \dots, W_{(t)}^{(L)}\right)$
    - Update $W^{(l)}$: $W_{(t+1)}^{(l)} = W_{(t)}^{(l)} - \eta_0 G^{(l)}$
  - Increment $t$: $t = t + 1$
- Output: $W_{(t)}^{(1)}, \dots, W_{(t)}^{(L)}$

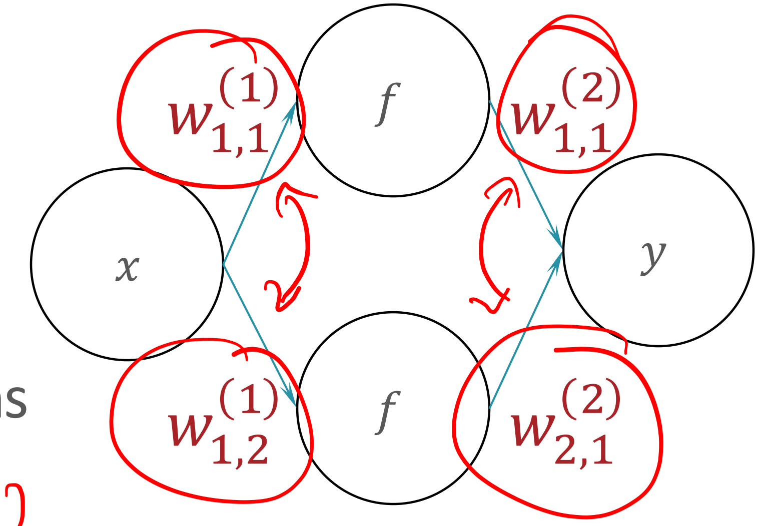
# Poll Question 2

- Suppose you are training a two-layer (one-hidden layer) neural network with sigmoid activations for binary classification.




- True or False: There is a unique set of parameters that maximizes the likelihood of the dataset above.

A. TOXIC B. True C. False




non-convex objective function!

# Neural Network Learning Objectives

You should be able to…

1. Explain the biological motivations for a neural network
2. Combine simpler models (e.g. linear regression, binary logistic regression, multinomial logistic regression) as components to build up feed-forward neural network architectures
3. Explain the reasons why a neural network can model nonlinear decision boundaries for classification
4. Compare and contrast feature engineering with learning features
5. Identify (some of) the options available when designing the architecture of a neural network
6. Implement a feed-forward neural network