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

Matt Gormley & Henry Chai

2/17/25

Front Matter

- Announcements
  - Exam 1 on 2/17 (today!) from 7 PM - 9 PM
    - Make sure you check the seating chart (on Piazza) so that you know where you're going tonight!
  - Homework 4 released 2/17 (today!), due 2/26 at 11:59 PM

Motivation: Regularization

- **Occam's Razor:** prefer the simplest hypothesis

- What does it mean for a hypothesis (or model) to be **simple**?
  1. small number of features (**model selection**)
  2. small number of "important" features (**shrinkage**)

Regularization

- **Given** objective function: J(θ)
- **Goal** is to find: $\hat{\boldsymbol{\theta}} = \underset{\boldsymbol{\theta}}{\operatorname{argmin}}\, J(\boldsymbol{\theta}) + \lambda r(\boldsymbol{\theta})$

- **Key idea:** Define regularizer r(θ) s.t. we tradeoff between fitting the data and keeping the model simple
- **Choose form of r(θ):**
  - Example: q-norm (usually p-norm): $\|\boldsymbol{\theta}\|_q = \left(\sum_{m=1}^{M} |\theta_m|^q\right)^{\frac{1}{q}}$

q	$r(\boldsymbol{\theta})$	**yields parameters that are...**	**name**	**optimization notes**
0	$\|\|\boldsymbol{\theta}\|\|_0 = \sum \mathbb{1}(\theta_m \neq 0)$	zero values	L0 reg.	no good computational solutions
1	$\|\|\boldsymbol{\theta}\|\|_1 = \sum \|\theta_m\|$	zero values	L1 reg.	subdifferentiable
2	$(\|\|\boldsymbol{\theta}\|\|_2)^2 = \sum \theta_m^2$	small values	L2 reg.	differentiable

Regularization Examples

Add an **L2 regularizer** to Linear Regression (aka. Ridge Regression)

$$J_{\text{RR}}(\boldsymbol{\theta}) = J(\boldsymbol{\theta}) + \lambda||\boldsymbol{\theta}||_2^2$$
$$= \frac{1}{N}\sum_{i=1}^{N}\frac{1}{2}(\boldsymbol{\theta}^T\mathbf{x}^{(i)} - y^{(i)})^2 + \lambda\sum_{m=1}^{M}\theta_m^2$$

Add an **L1 regularizer** to Linear Regression (aka. LASSO)

$$J_{\text{LASSO}}(\boldsymbol{\theta}) = J(\boldsymbol{\theta}) + \lambda||\boldsymbol{\theta}||_1$$
$$= \frac{1}{N}\sum_{i=1}^{N}\frac{1}{2}(\boldsymbol{\theta}^T\mathbf{x}^{(i)} - y^{(i)})^2 + \lambda\sum_{m=1}^{M}|\theta_m|$$

Regularization Examples

Add an **L2 regularizer** to Logistic Regression

$$J'(\boldsymbol{\theta}) = J(\boldsymbol{\theta}) + \lambda||\boldsymbol{\theta}||_2^2$$

$$= \frac{1}{N}\sum_{i=1}^{N} -\log p(y^{(i)} \mid \mathbf{x}^{(i)}, \boldsymbol{\theta}) + \lambda\sum_{m=1}^{M}\theta_m^2$$

Add an **L1 regularizer** to Logistic Regression

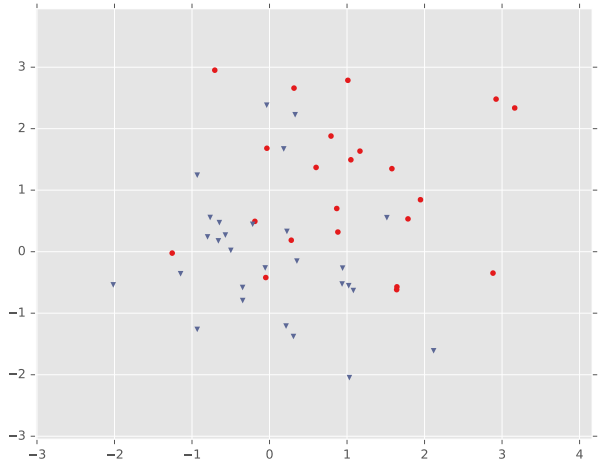
$$J'(\boldsymbol{\theta}) = J(\boldsymbol{\theta}) + \lambda||\boldsymbol{\theta}||_1$$

$$= \frac{1}{N}\sum_{i=1}^{N} -\log p(y^{(i)} \mid \mathbf{x}^{(i)}, \boldsymbol{\theta}) + \lambda\sum_{m=1}^{M}|\theta_m|$$

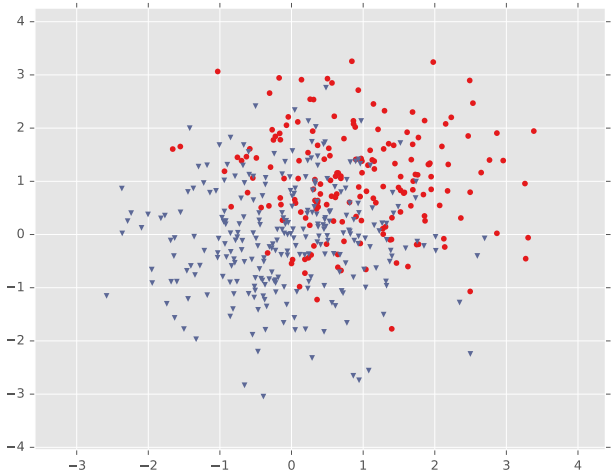
REGULARIZATION EXAMPLE: LOGISTIC REGRESSION

Example: Logistic Regression

Training Data

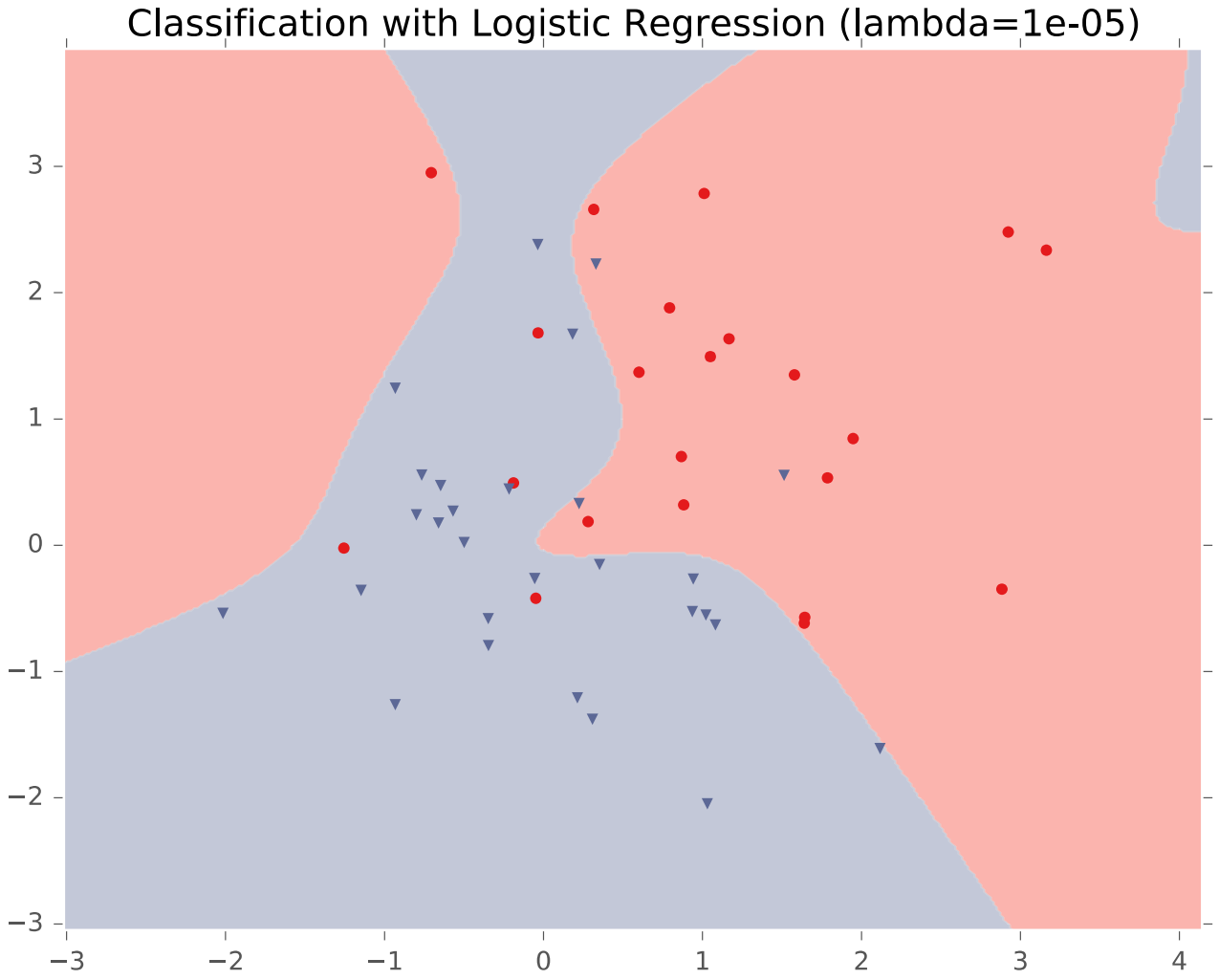


Test Data

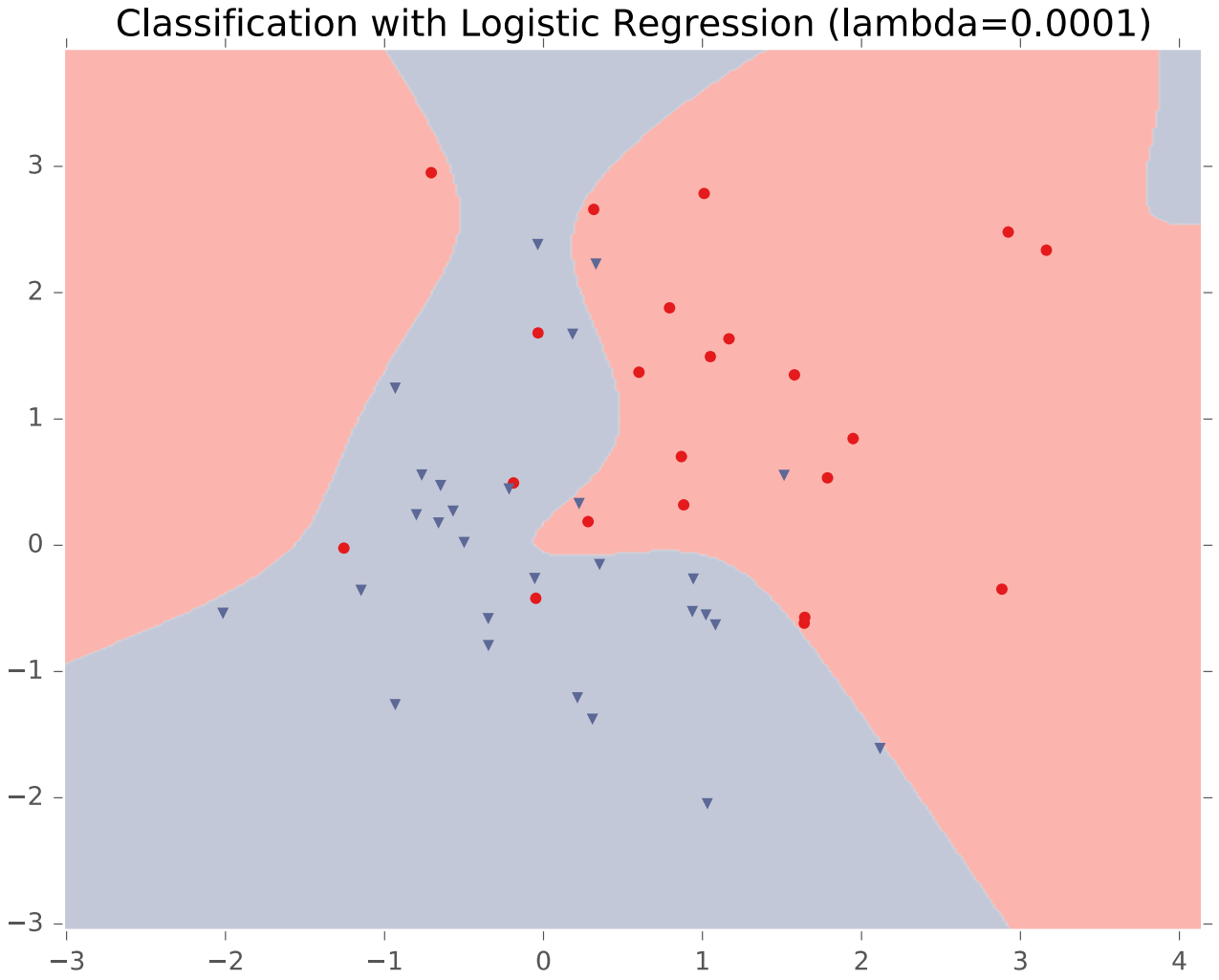


- For this example, we construct **nonlinear features** (i.e. feature engineering)
- Specifically, we add **polynomials up to order 9** of the two original features x_1 and x_2
- Thus our classifier is **linear** in the **high-dimensional feature space**, but the decision boundary is **nonlinear** when visualized in **low-dimensions** (i.e. the original two dimensions)

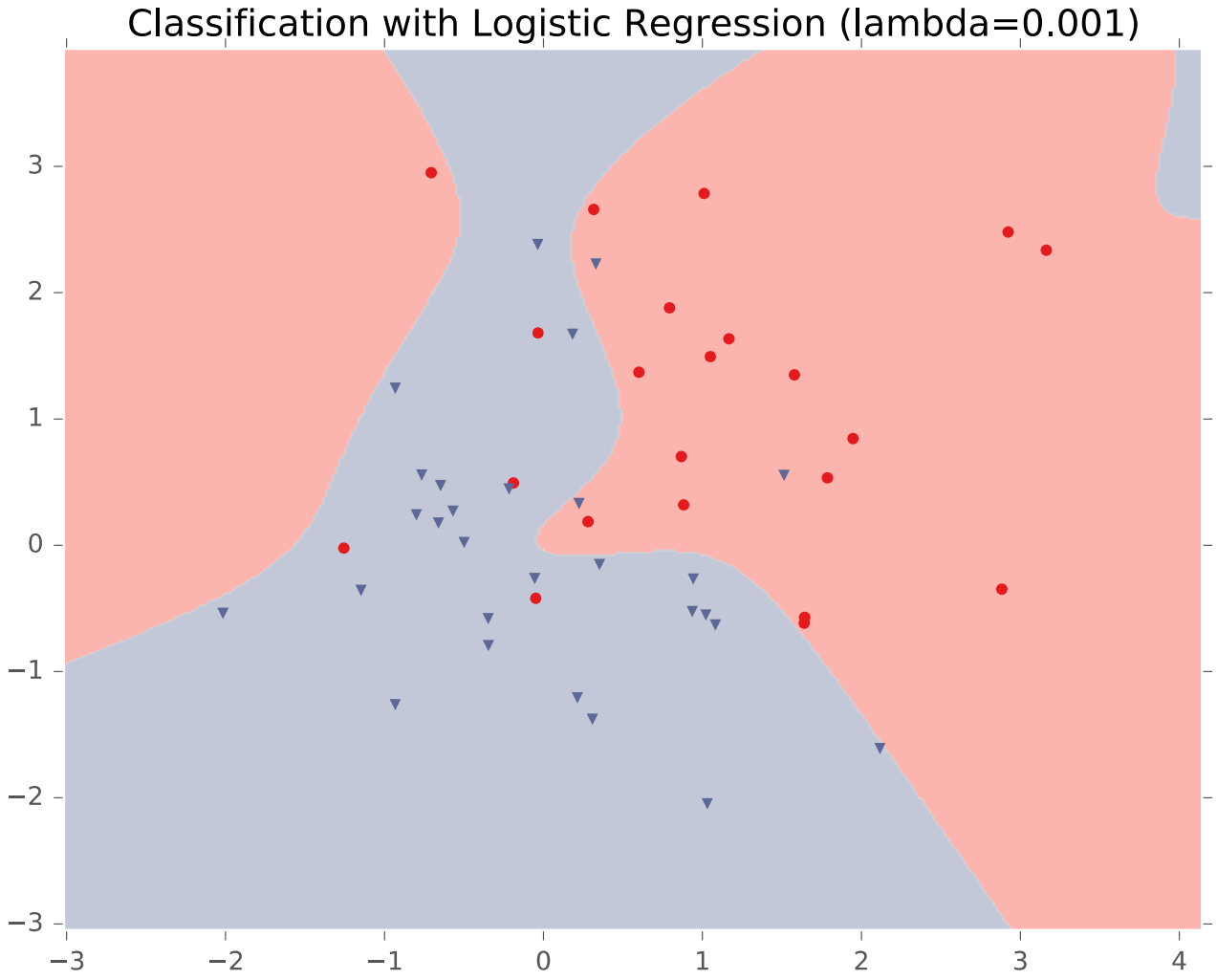
Example: Logistic Regression



Example: Logistic Regression



Example: Logistic Regression



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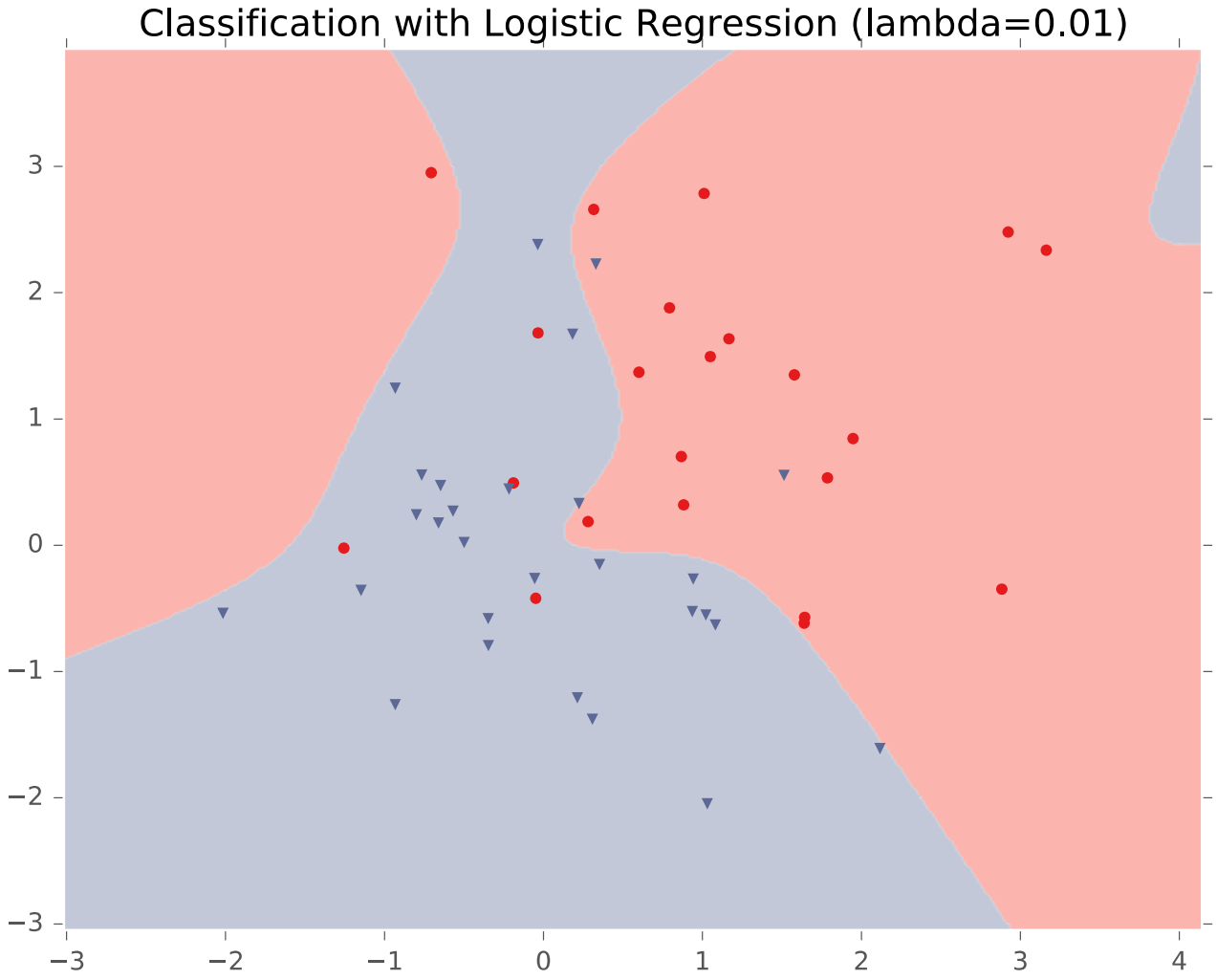

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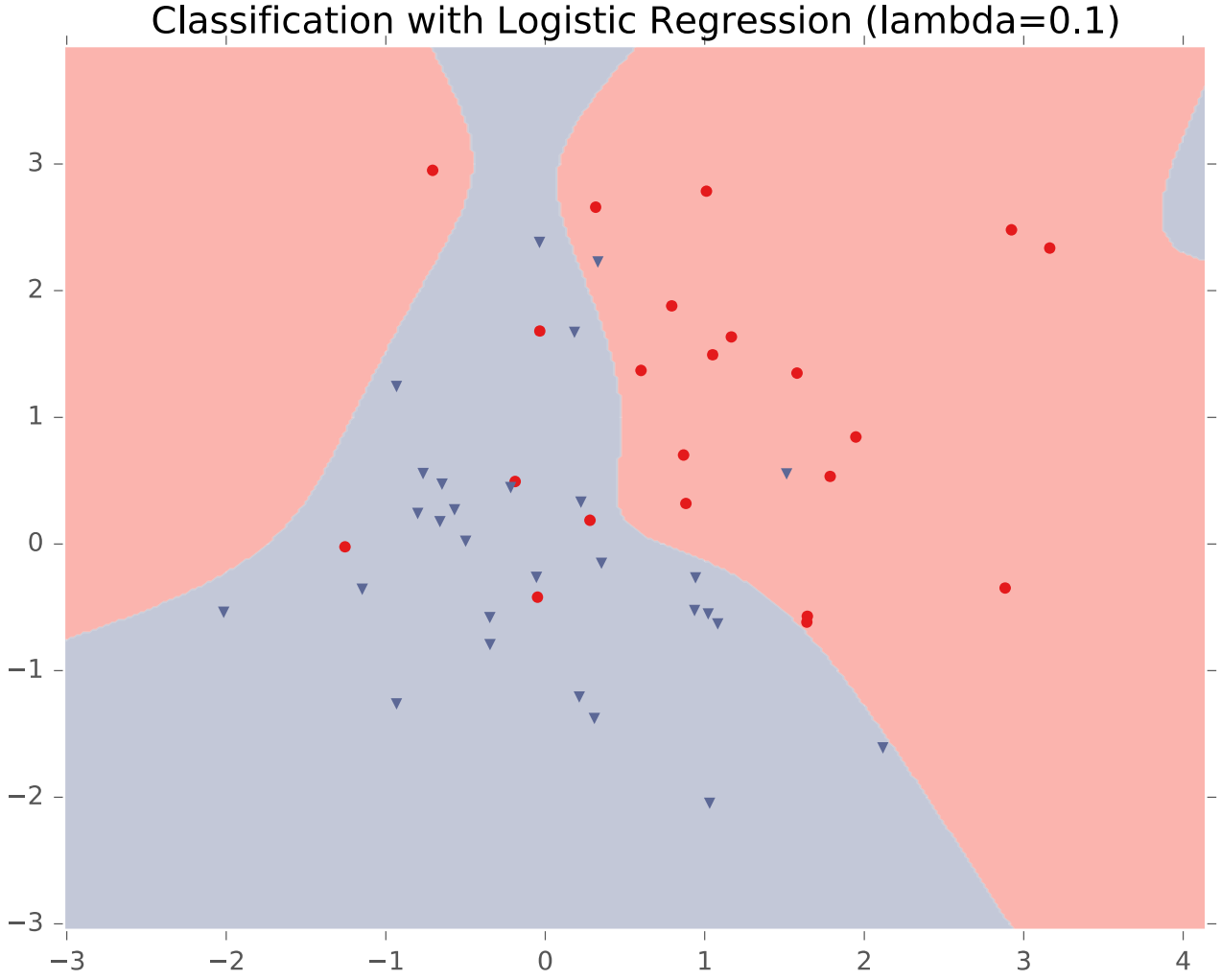

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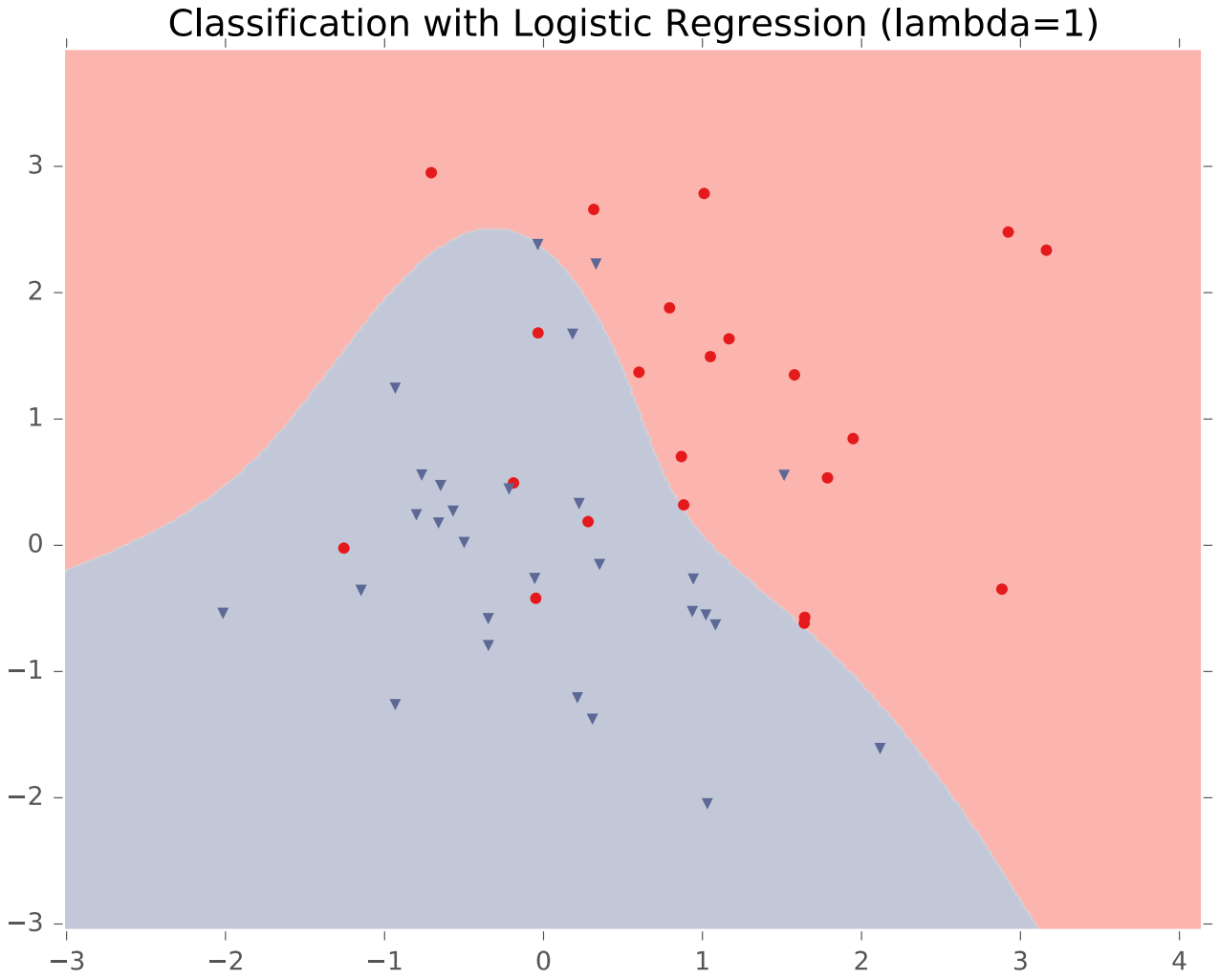

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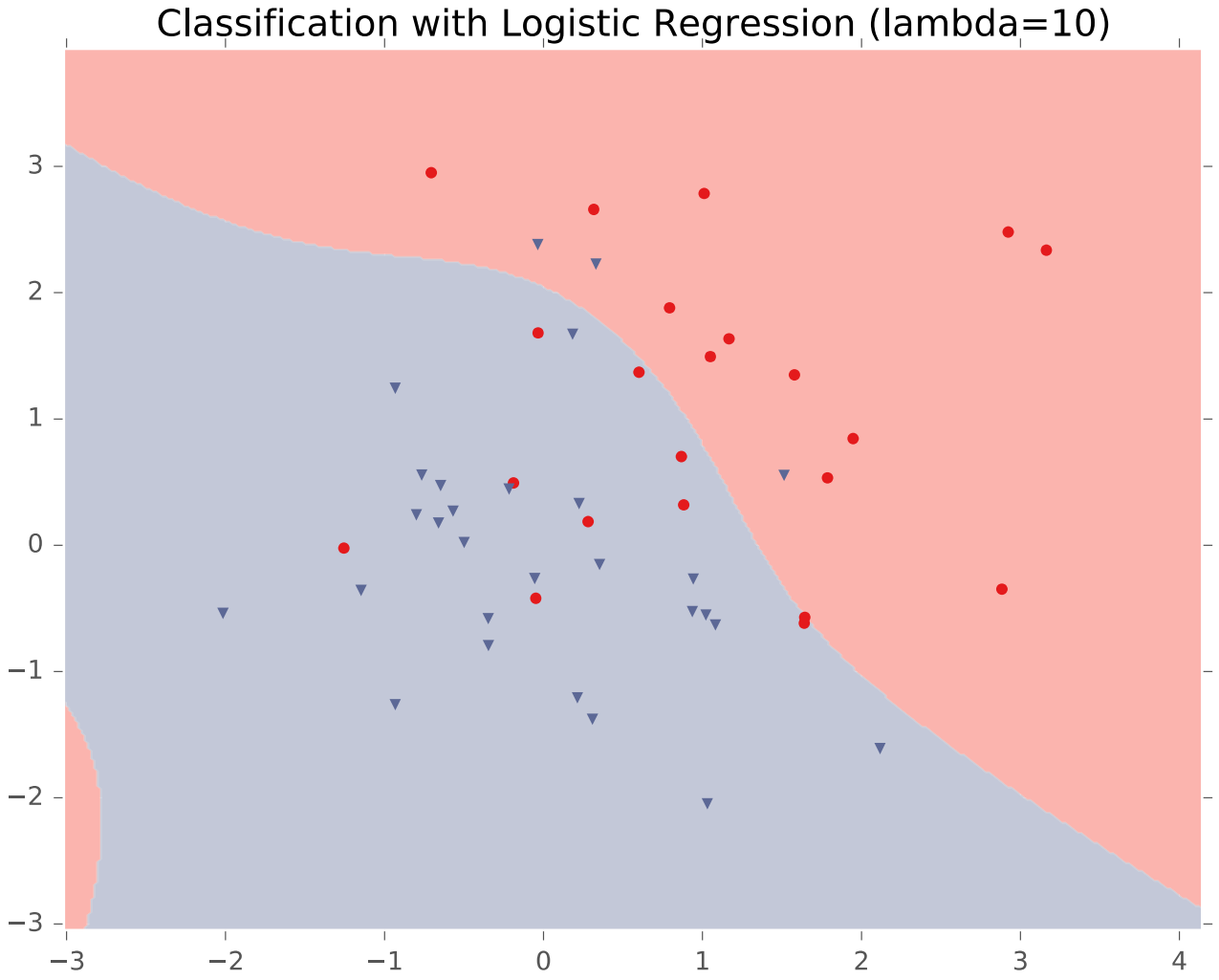

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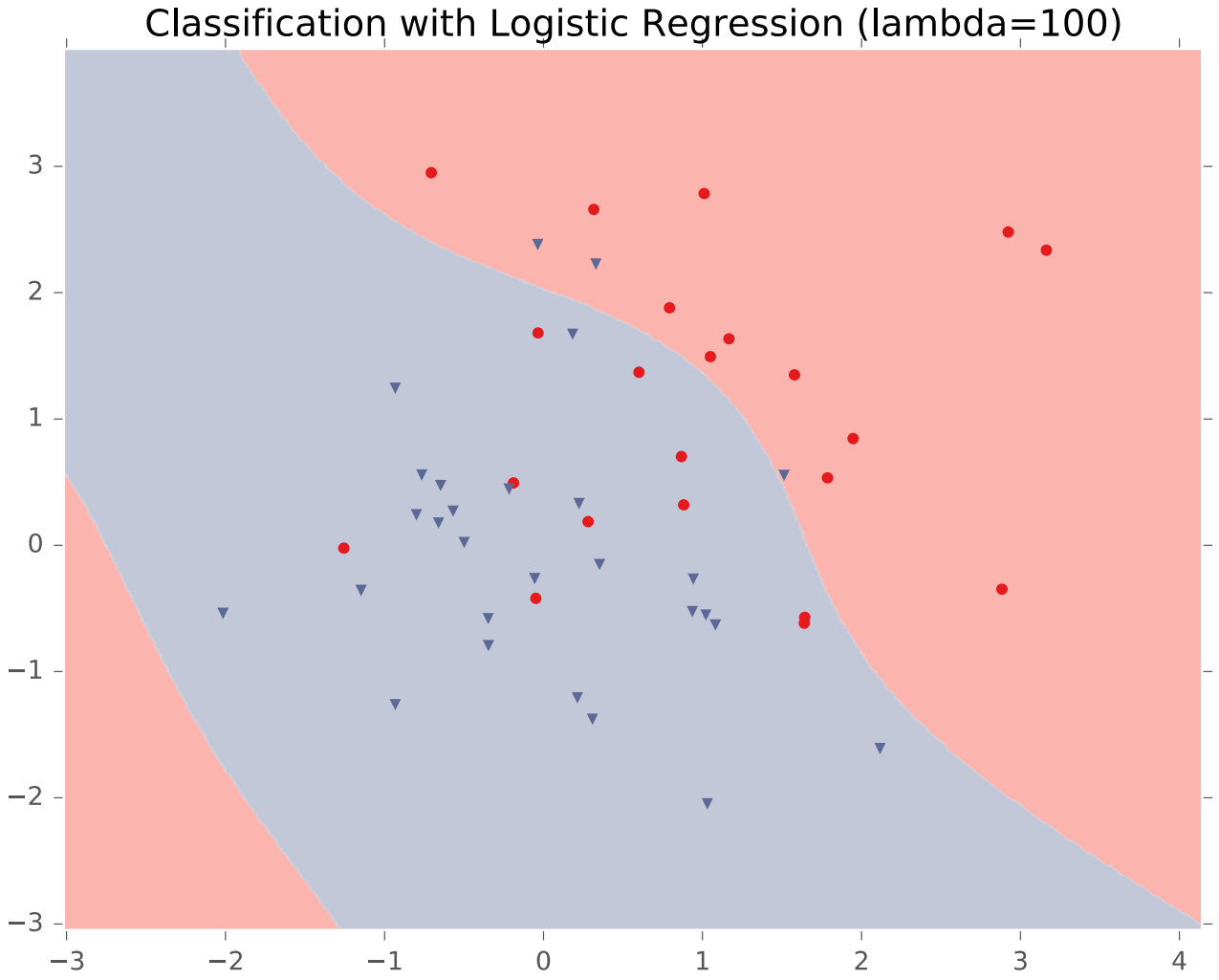

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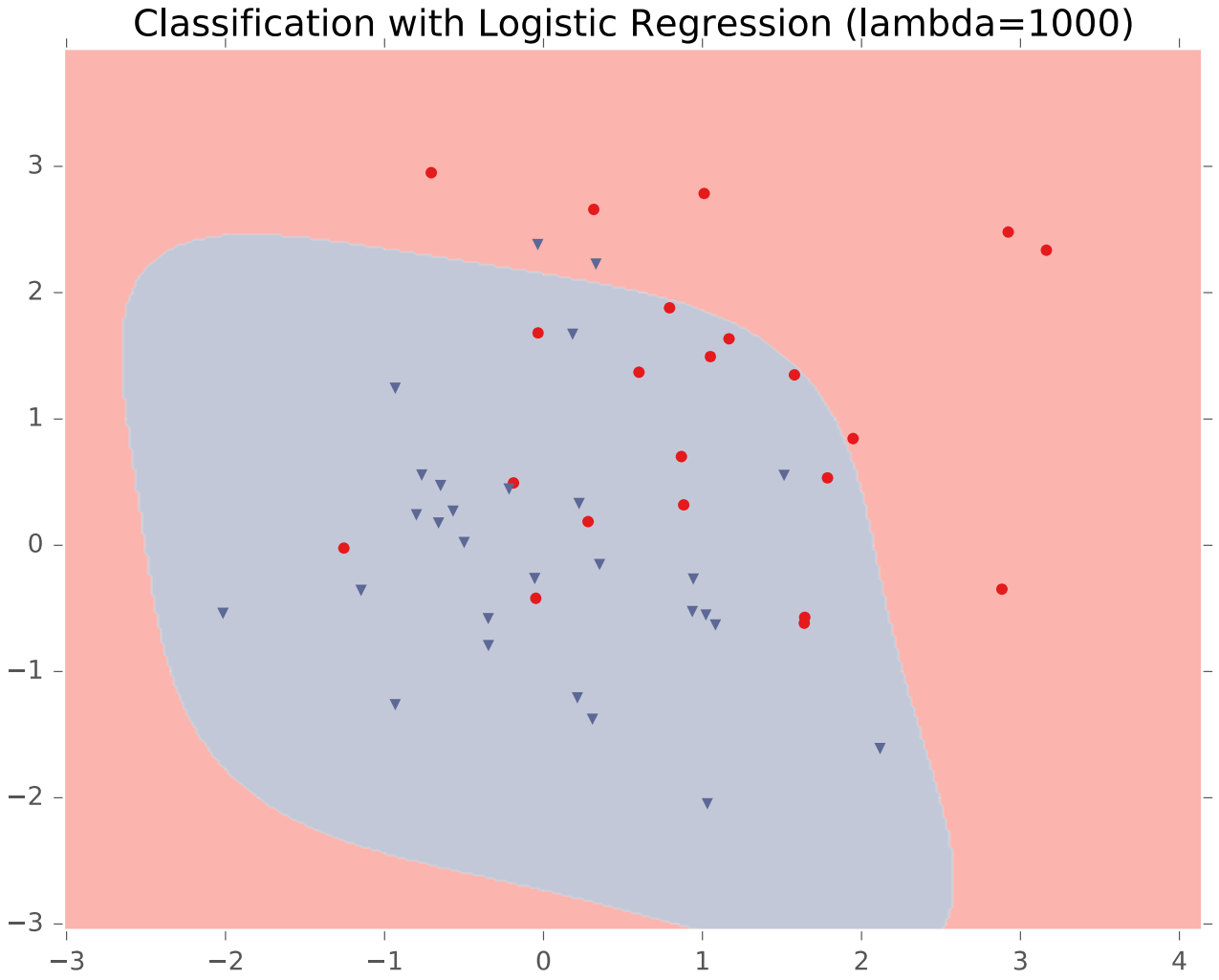

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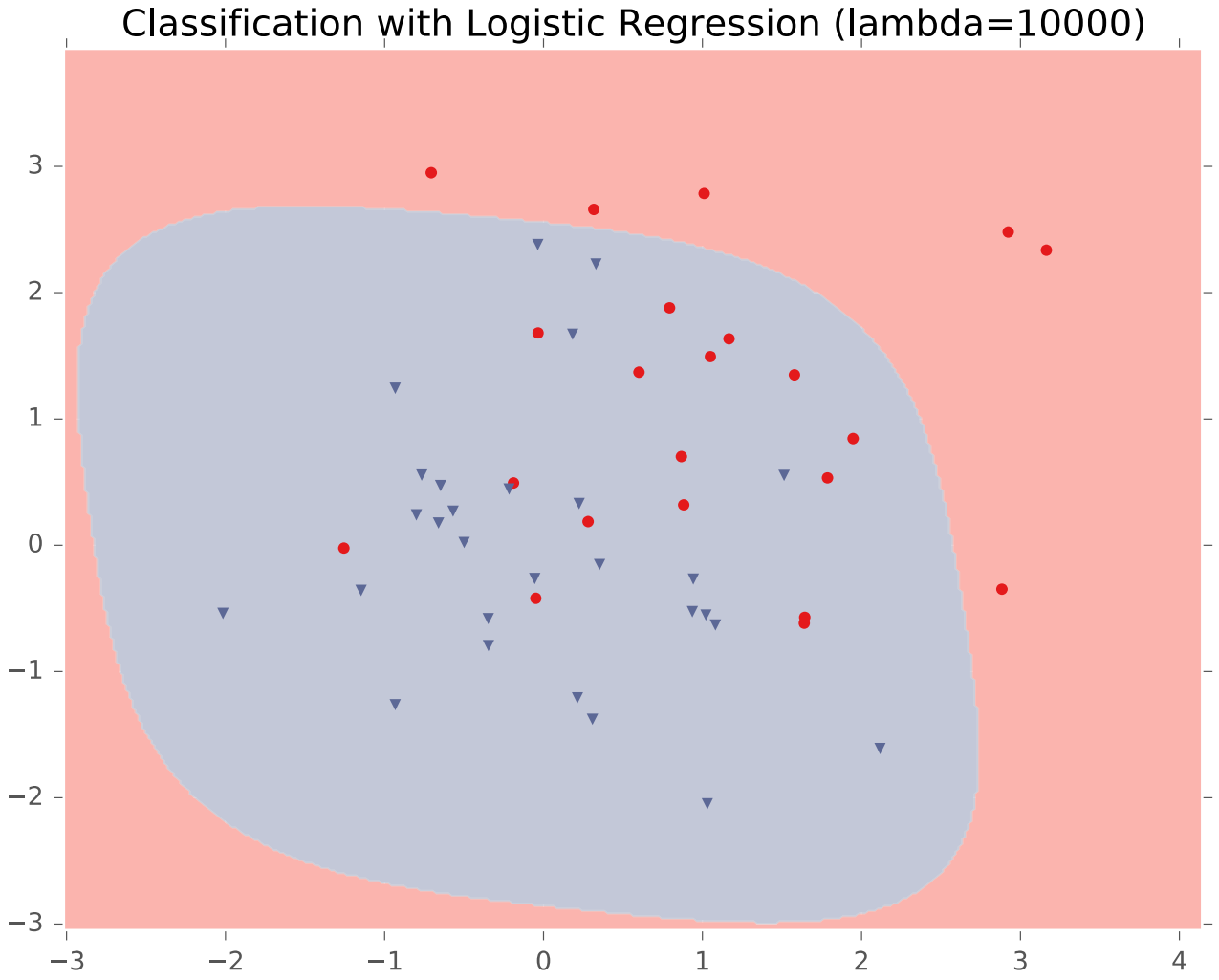

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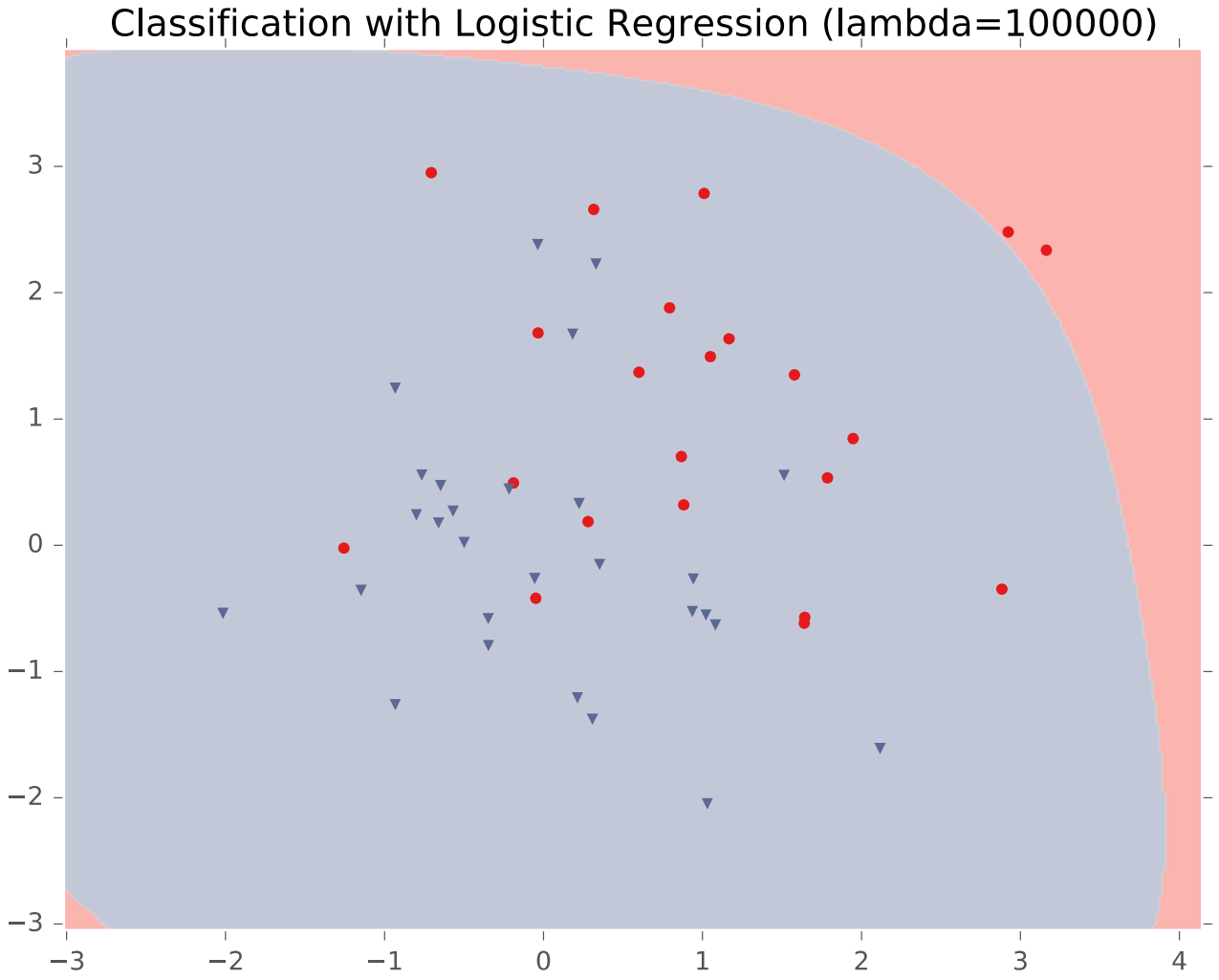

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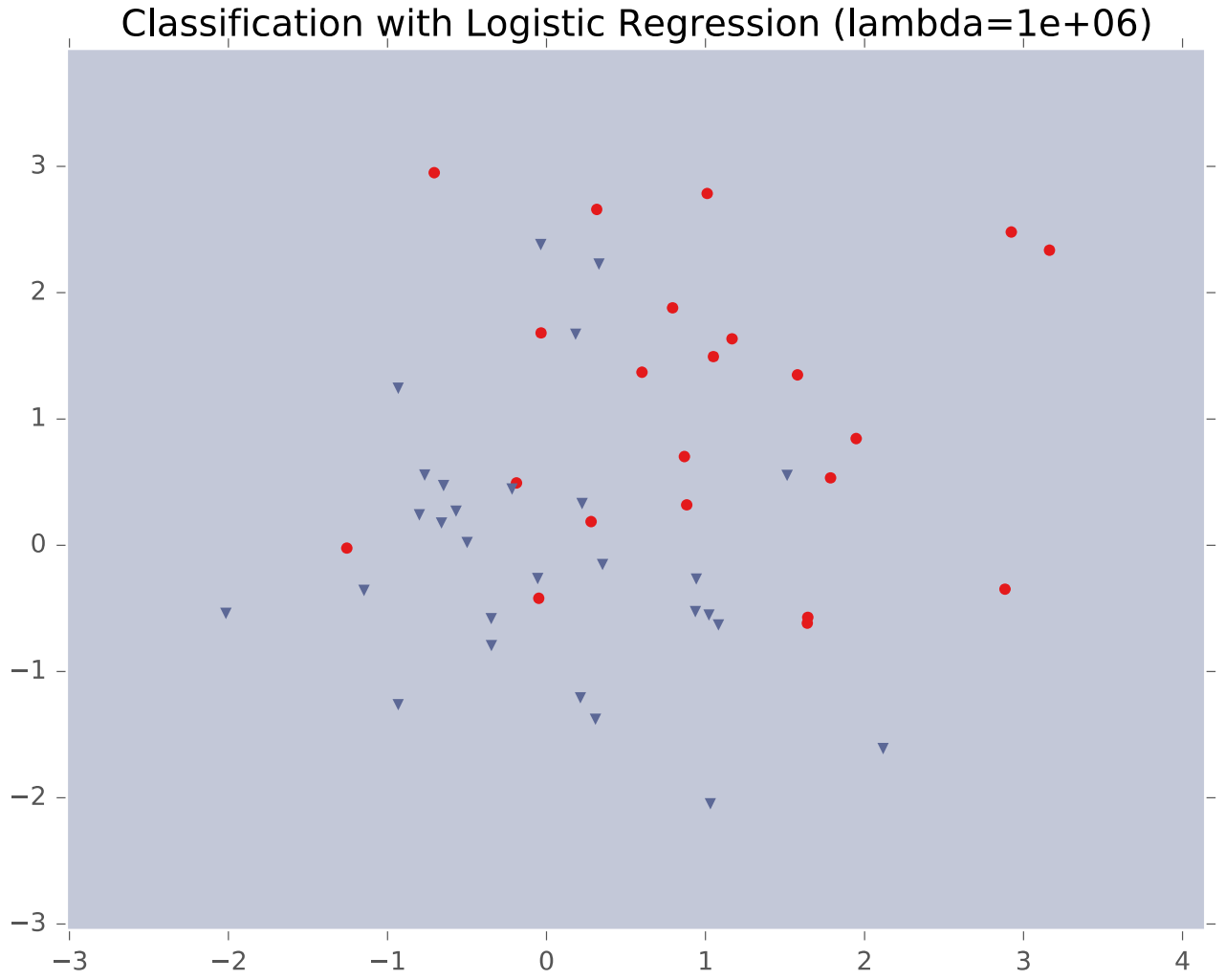

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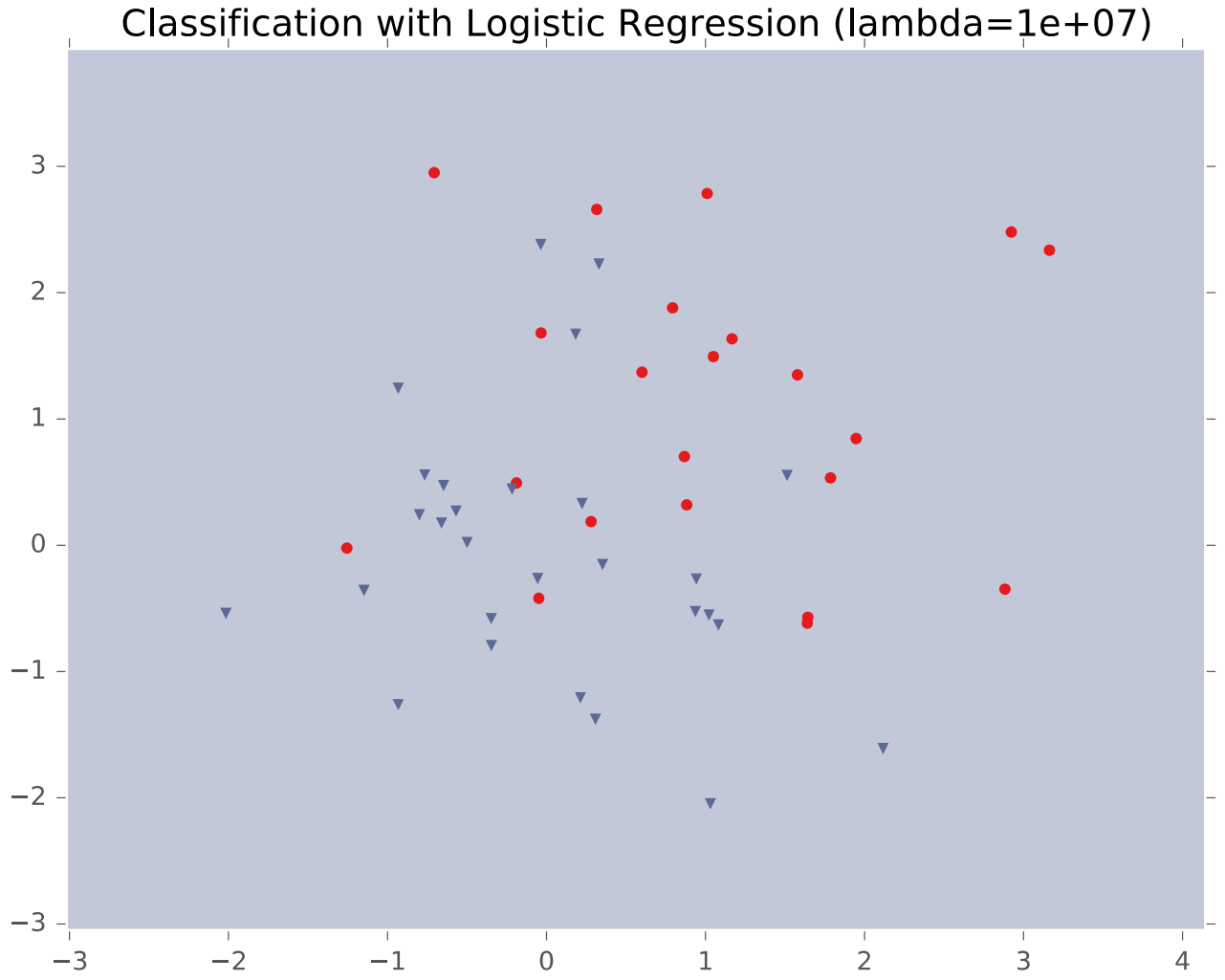

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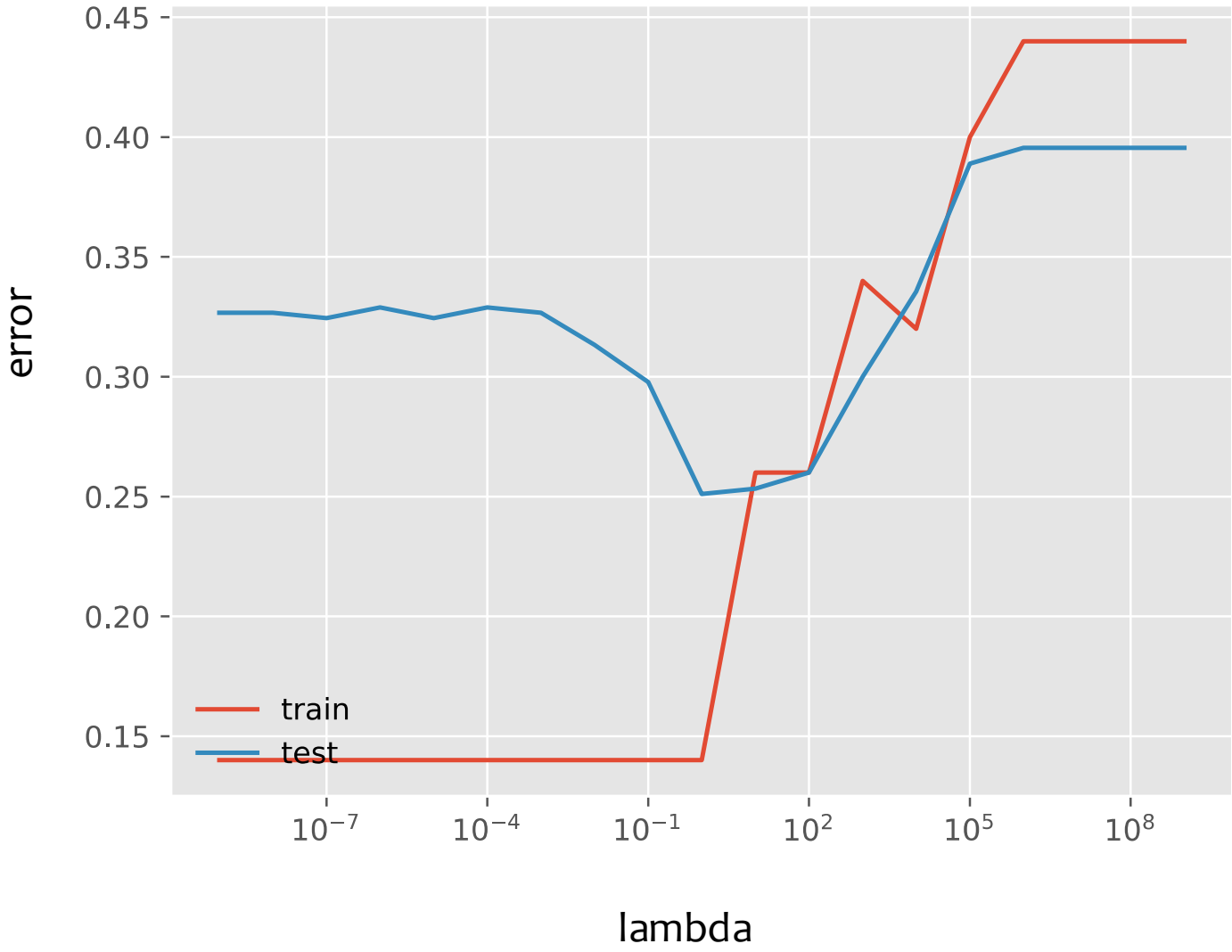


Regularization

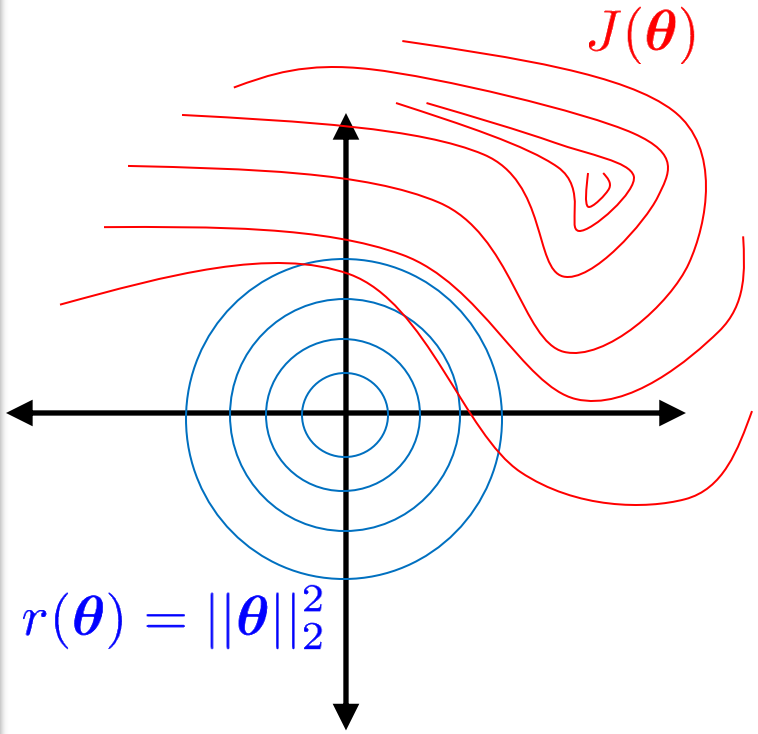
Poll Question 1:

Suppose we are minimizing J'(θ) where

$$J'(\boldsymbol{\theta}) = J(\boldsymbol{\theta}) + \lambda r(\boldsymbol{\theta})$$

As λ increases, the minimum of J'(θ) will…

A. …move towards the midpoint between J(θ) and r(θ)
B. …move towards the minimum of J(θ)
C. …move towards the minimum of r(θ)
D. …move towards a theta vector of positive infinities
E. …move towards a theta vector of negative infinities
F. …stay the same **(TOXIC)**



Regularization: Best Practices

Don't Regularize the Bias (Intercept) Parameter!

- In our models so far, the bias / intercept parameter is usually denoted by θ_0 -- that is, the parameter for which we fixed $x_0 = 1$
- Regularizers always avoid penalizing this bias / intercept parameter
- Why? Because otherwise the learning algorithms wouldn't be invariant to a shift in the y-values

Standardizing Data

- It's common to *standardize* each feature by subtracting its mean and dividing by its standard deviation
- For regularization, this helps all the features be penalized in the same units
  (e.g. convert both centimeters and kilometers to z-scores)

Takeaways

1. **Nonlinear basis functions** allow **linear models** (e.g. Linear Regression, Logistic Regression) to capture **nonlinear** aspects of the original input
2. Nonlinear features **require no changes to the model** (i.e. just preprocessing)
3. **Regularization** helps to avoid **overfitting**

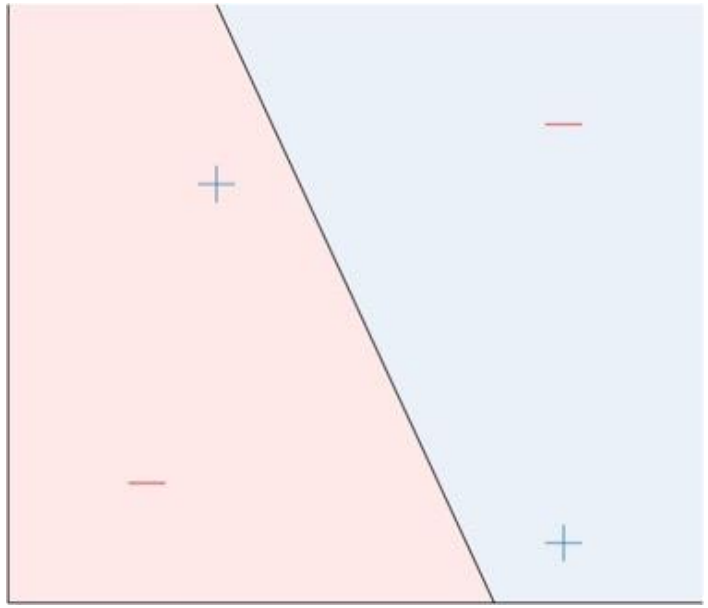
Feature Engineering / Regularization Objectives

You should be able to…

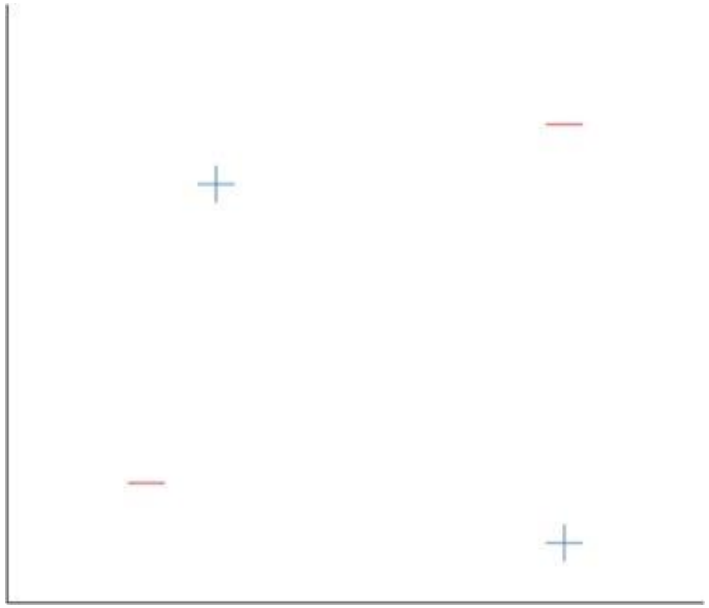
- Engineer appropriate features for a new task
- Use feature selection techniques to identify and remove irrelevant features
- Identify when a model is overfitting
- Add a regularizer to an existing objective in order to combat overfitting
- Explain why we should **not** regularize the bias term
- Convert linearly inseparable dataset to a linearly separable dataset in higher dimensions
- Describe feature engineering in common application areas

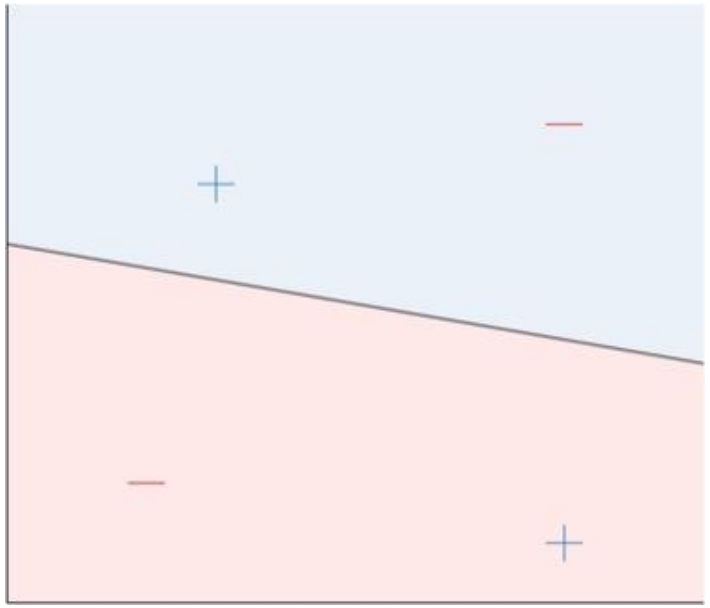
Biological Neural Network

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



h_1

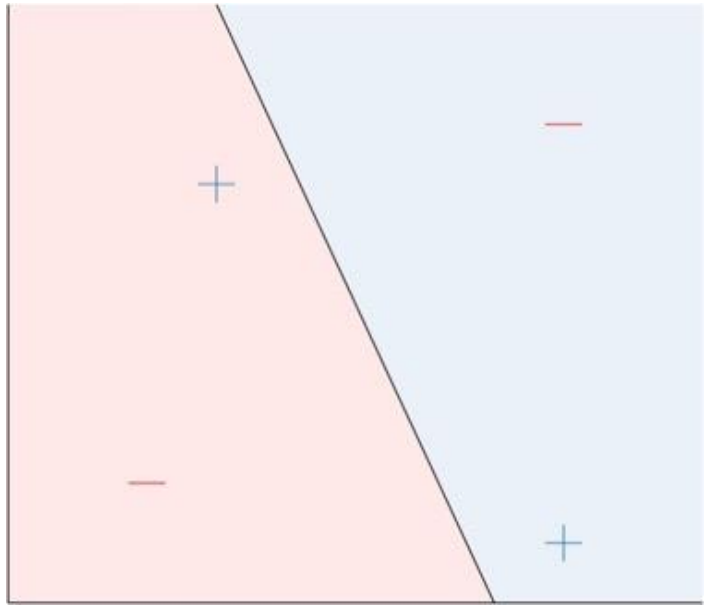




h_2

Perceptrons

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



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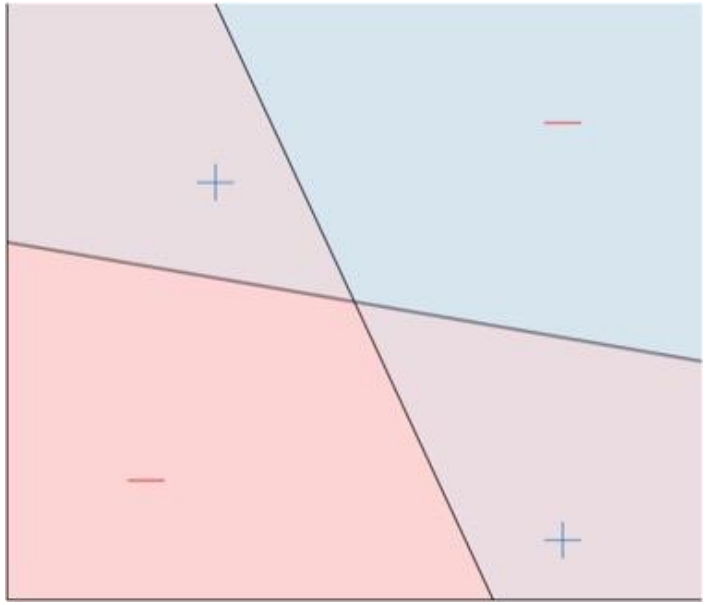
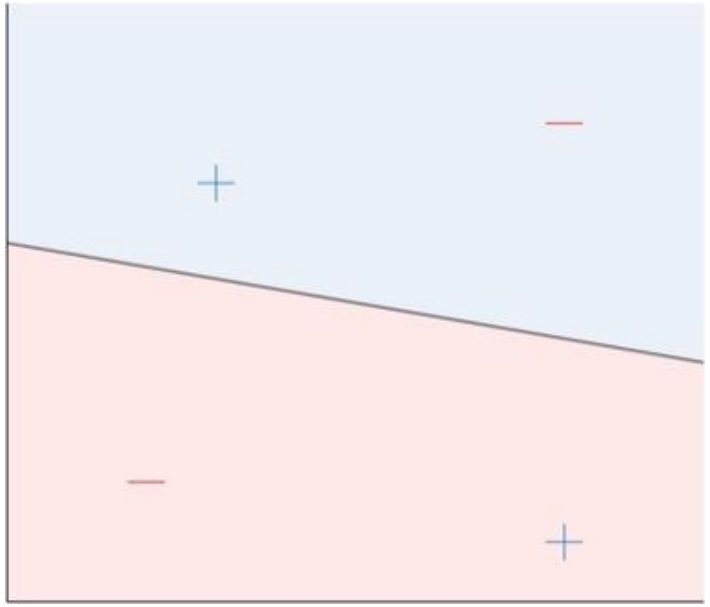


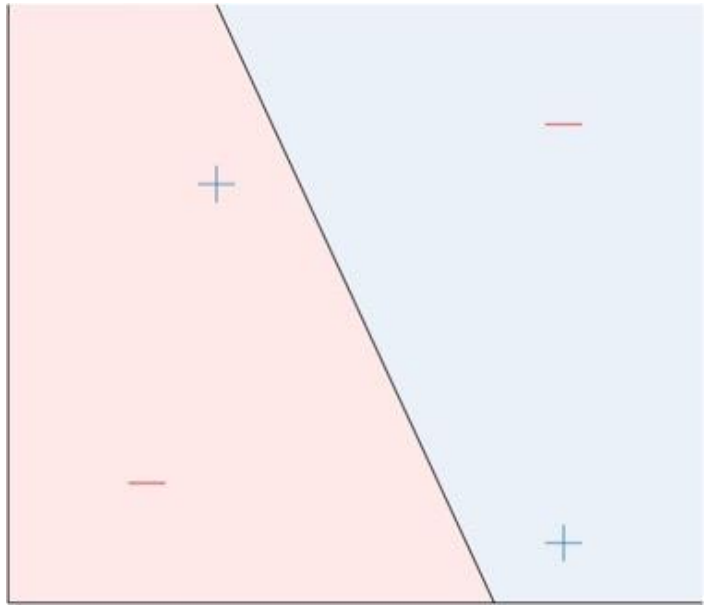
h_1

h_2

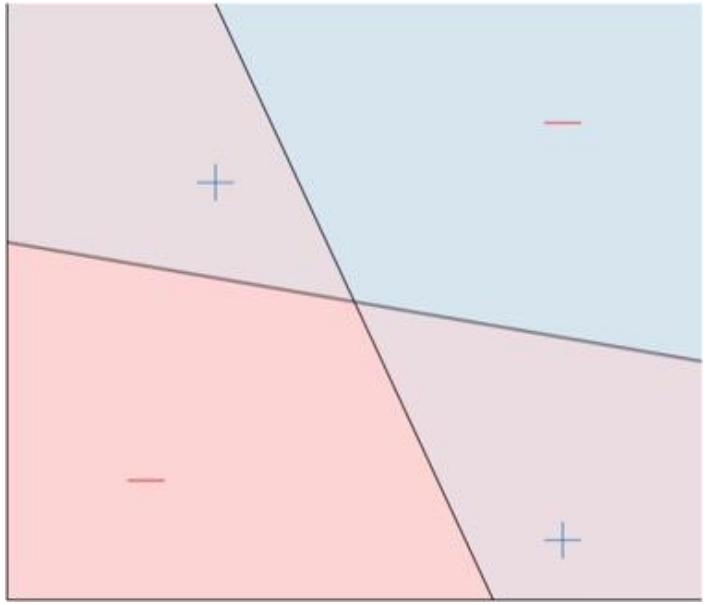


h_2

Combining Perceptrons

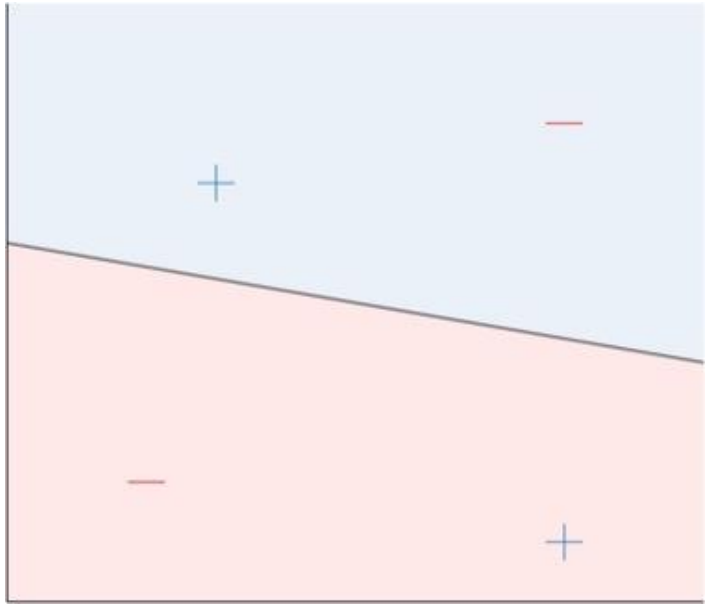


h_1



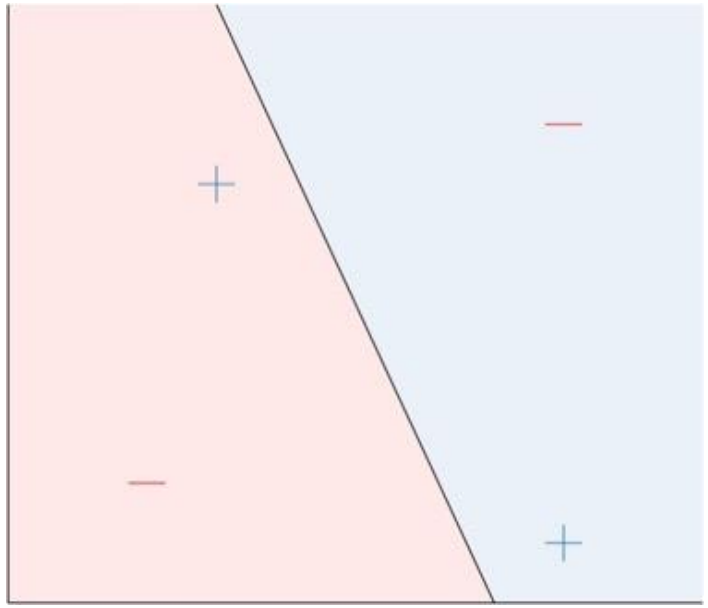
h_2

h_1



h_2

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



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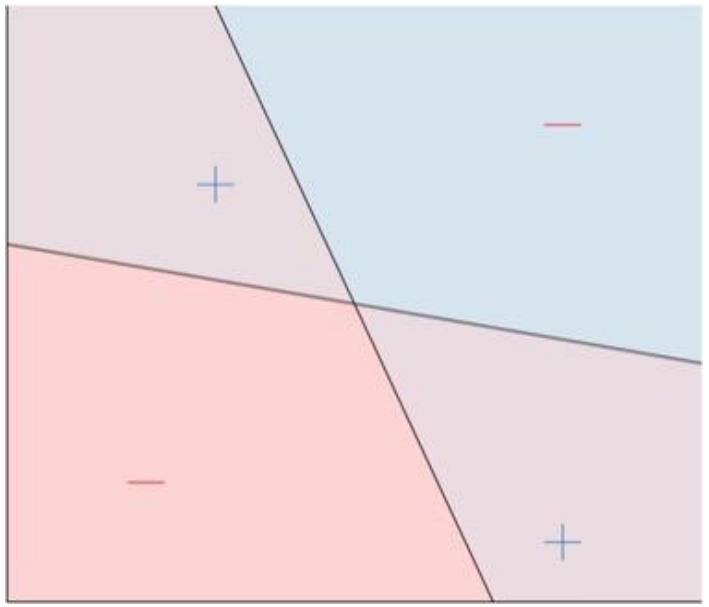
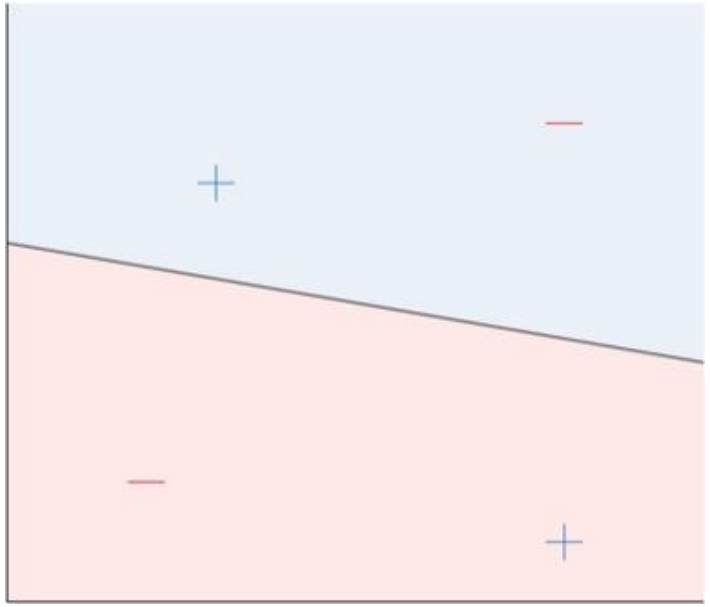


h_1

h_2



h_2

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

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

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- 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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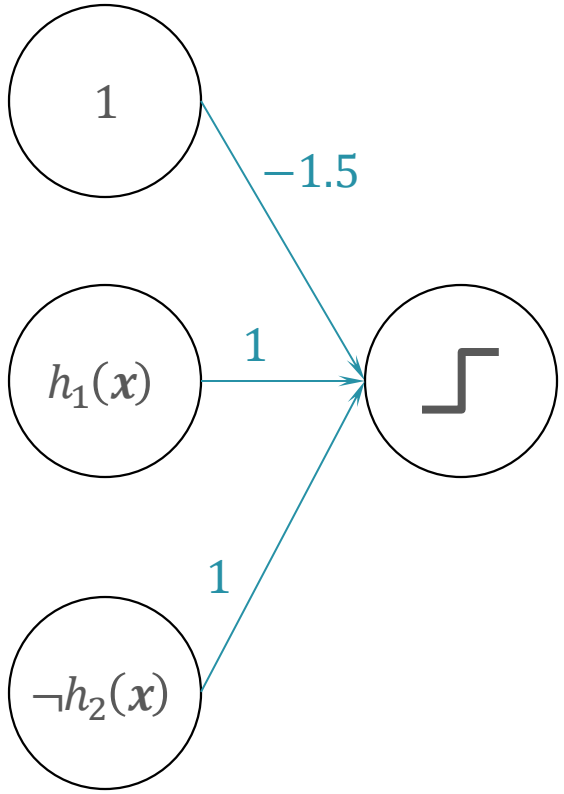

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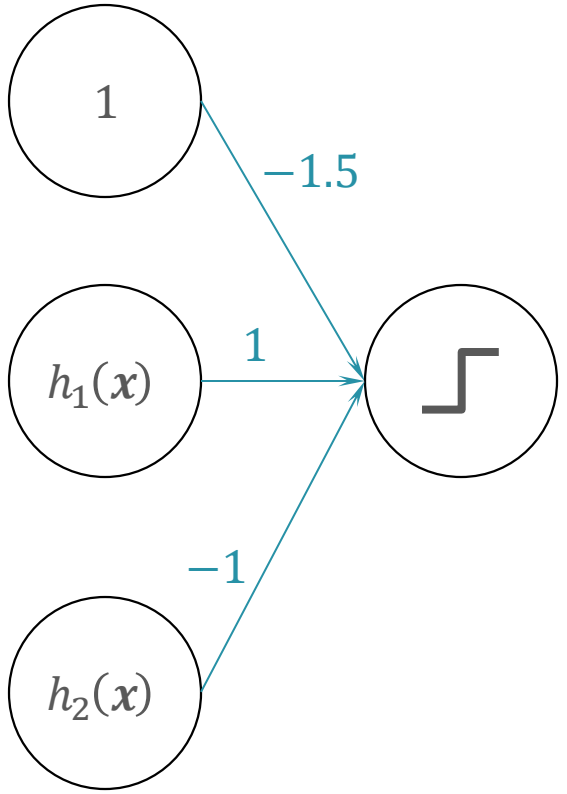

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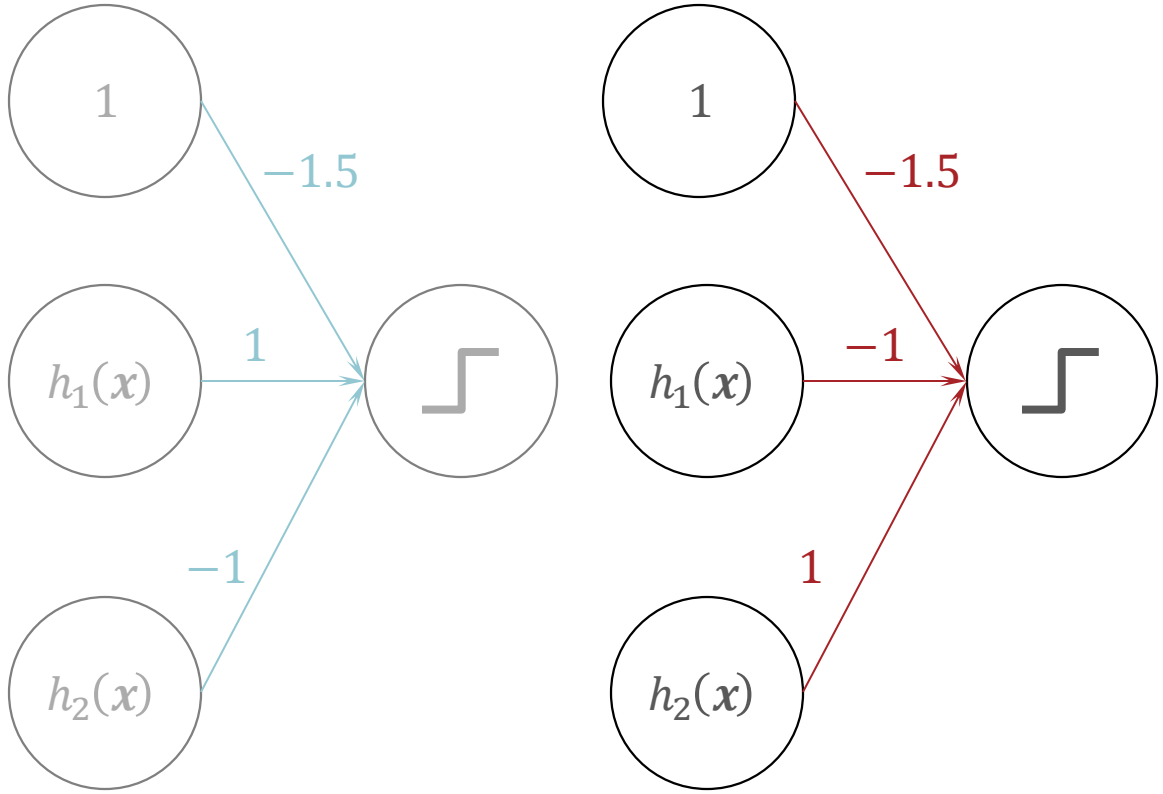

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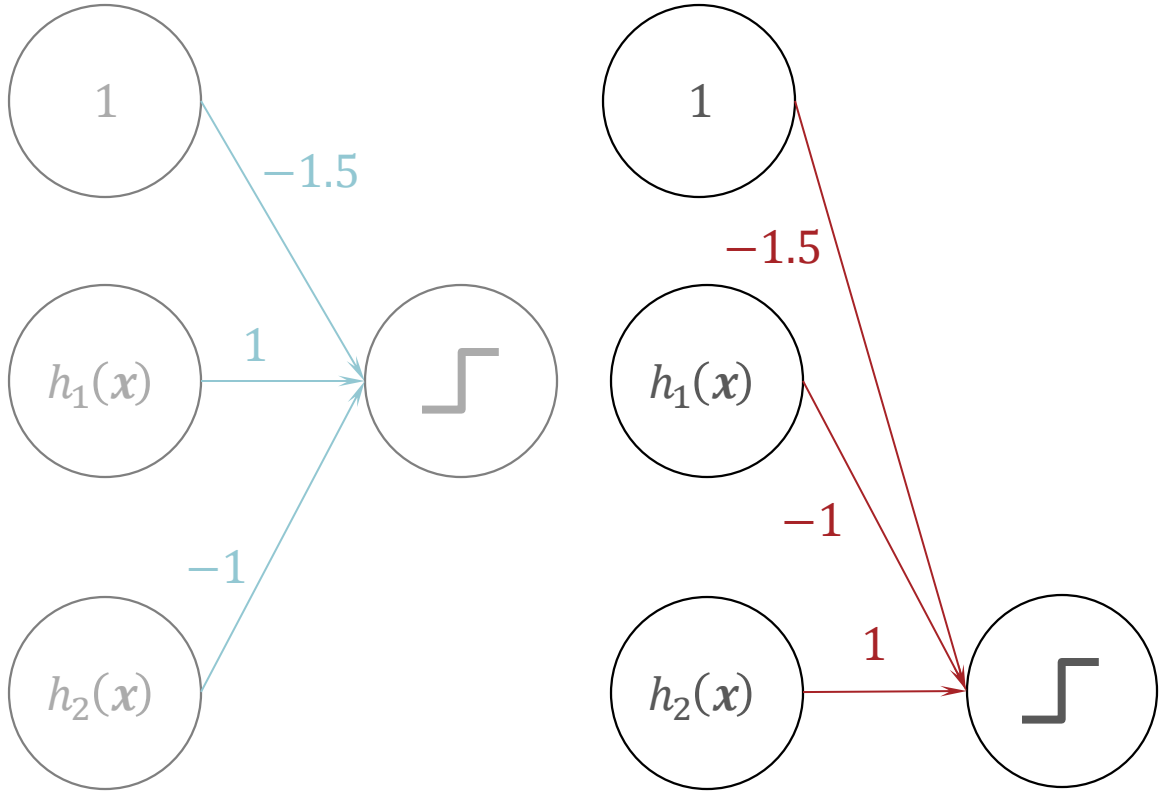

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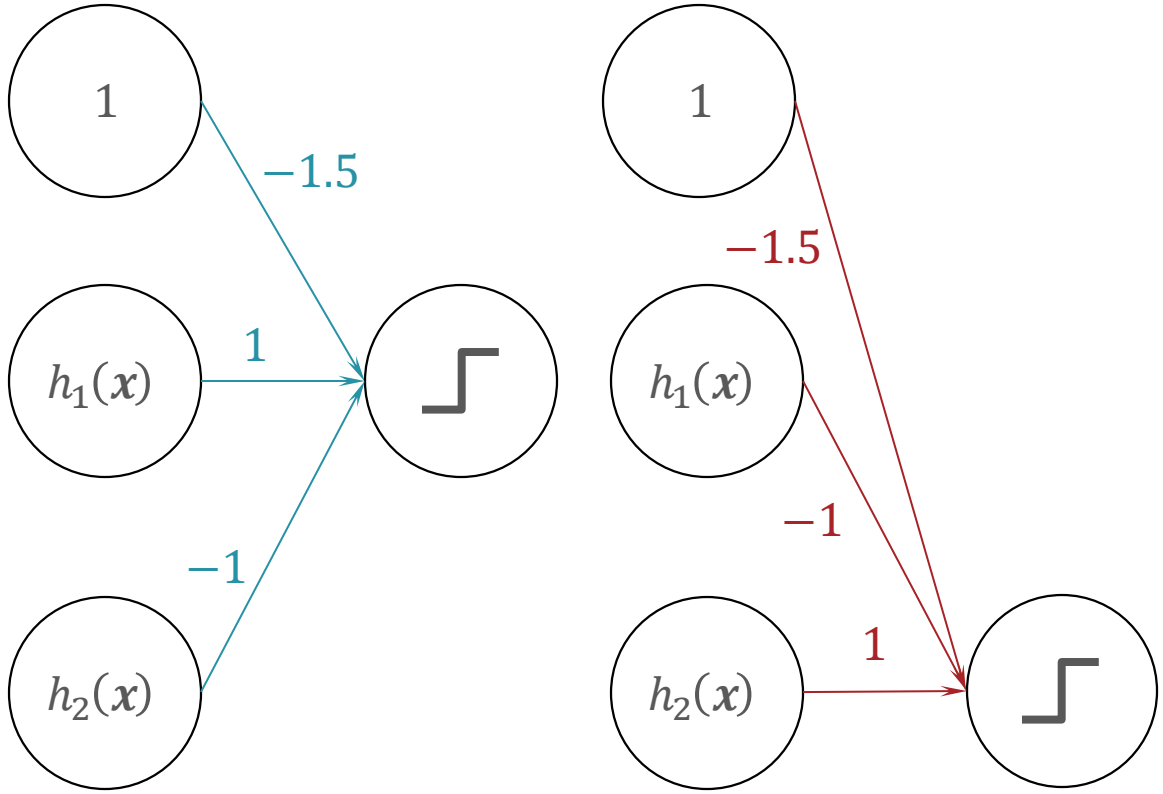

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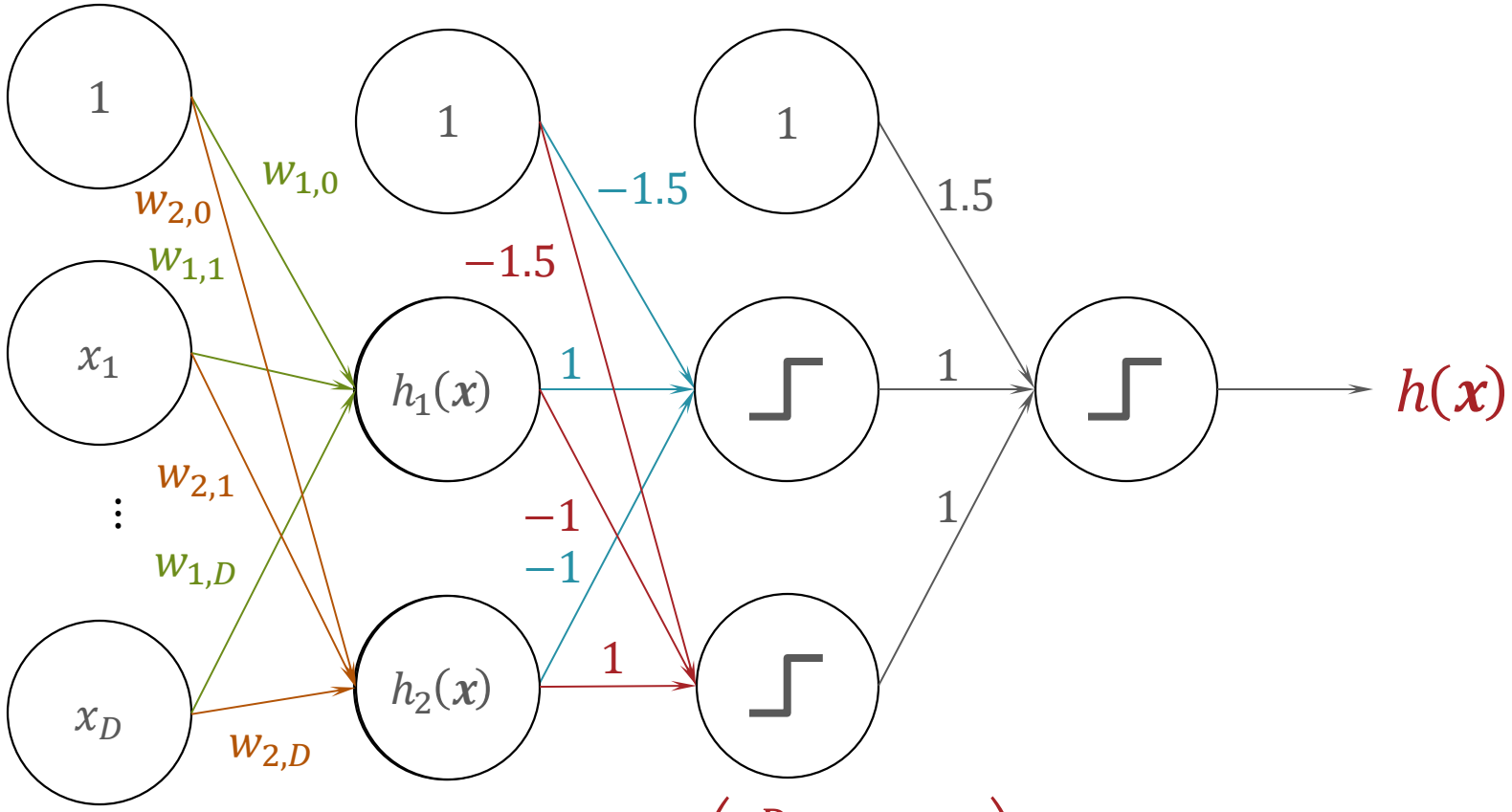
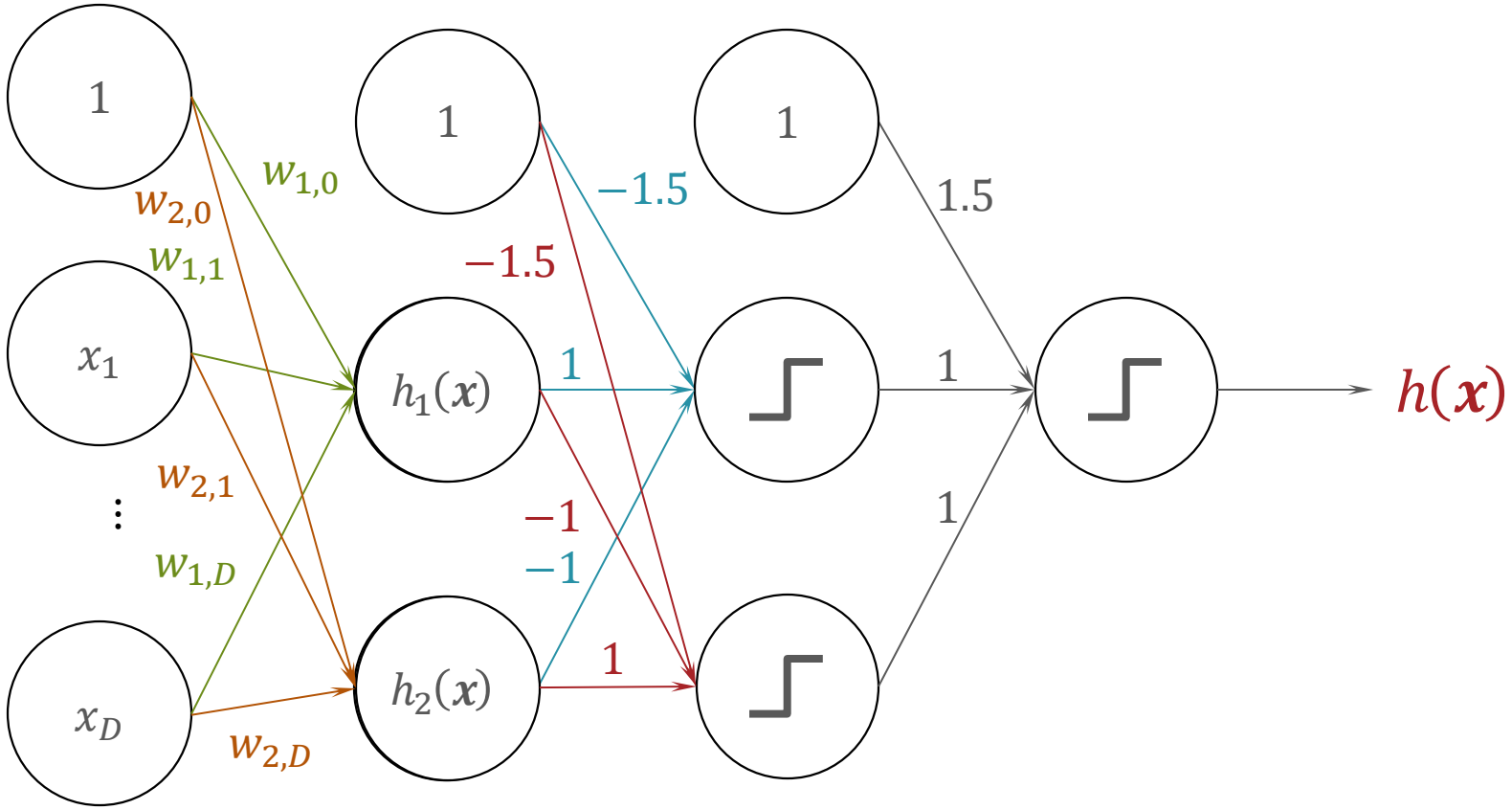


$$h_i(\boldsymbol{x}) = \text{sign}\big(\boldsymbol{w}_i^T \boldsymbol{x}\big) = \text{sign}\left(\sum_{d=0}^{D} w_{i,d}\, x_d\right)$$

Building a Network

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



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

Building a Network

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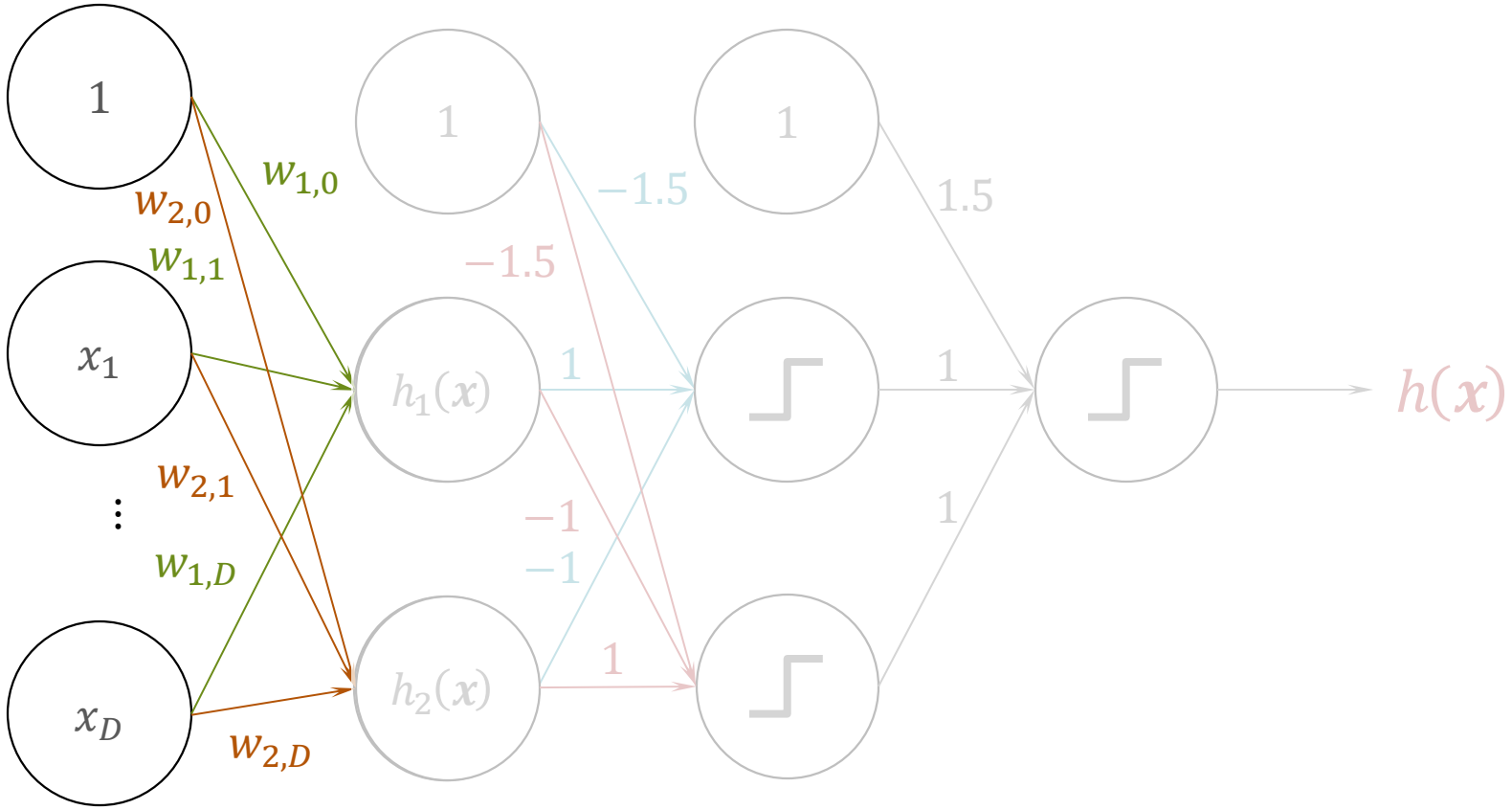
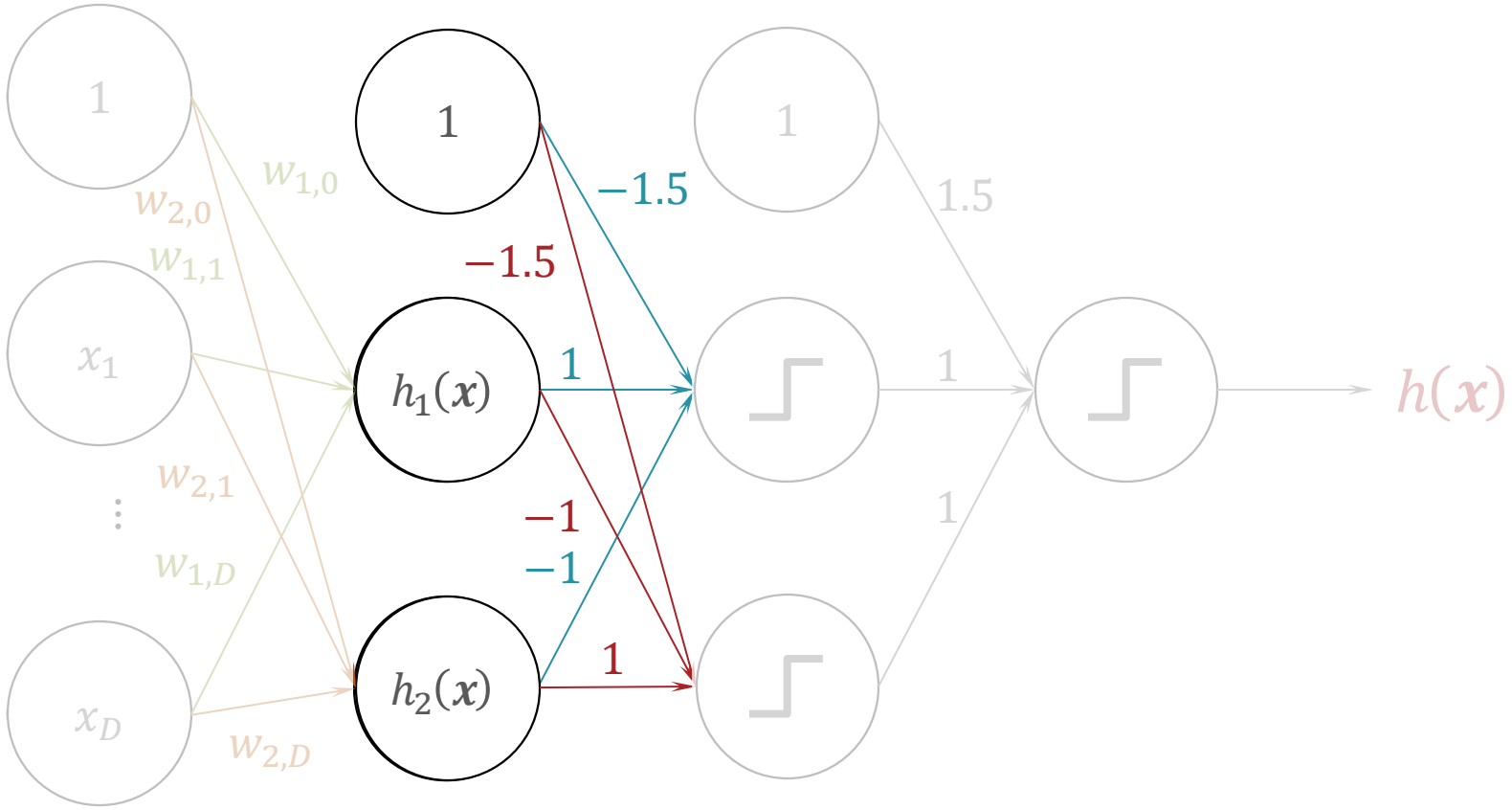


$$h(\boldsymbol{x}) = \text{sign}(\text{sign}(\text{sign}(\boldsymbol{w}_1^T\boldsymbol{x}) - \text{sign}(\boldsymbol{w}_2^T\boldsymbol{x}) - 1.5) + \text{sign}(-\text{sign}(\boldsymbol{w}_1^T\boldsymbol{x}) + \text{sign}(\boldsymbol{w}_2^T\boldsymbol{x}) - 1.5) + 1.5)$$

Building a Network

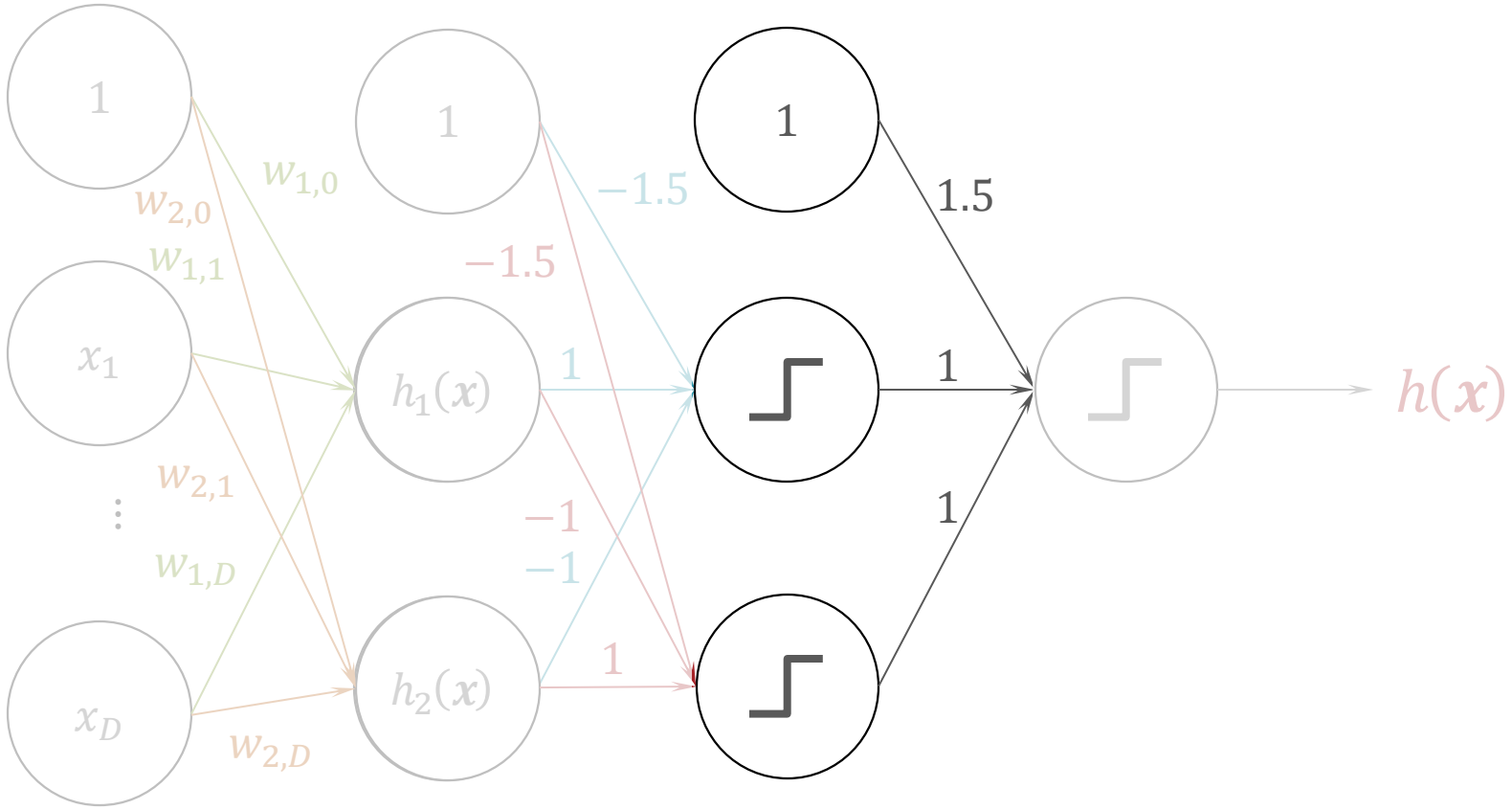
$$h(\boldsymbol{x}) = OR\Big(AND\big(h_1(\boldsymbol{x}), \neg h_2(\boldsymbol{x})\big), AND\big(\neg h_1(\boldsymbol{x}), h_2(\boldsymbol{x})\big)\Big)$$



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

Building a Network

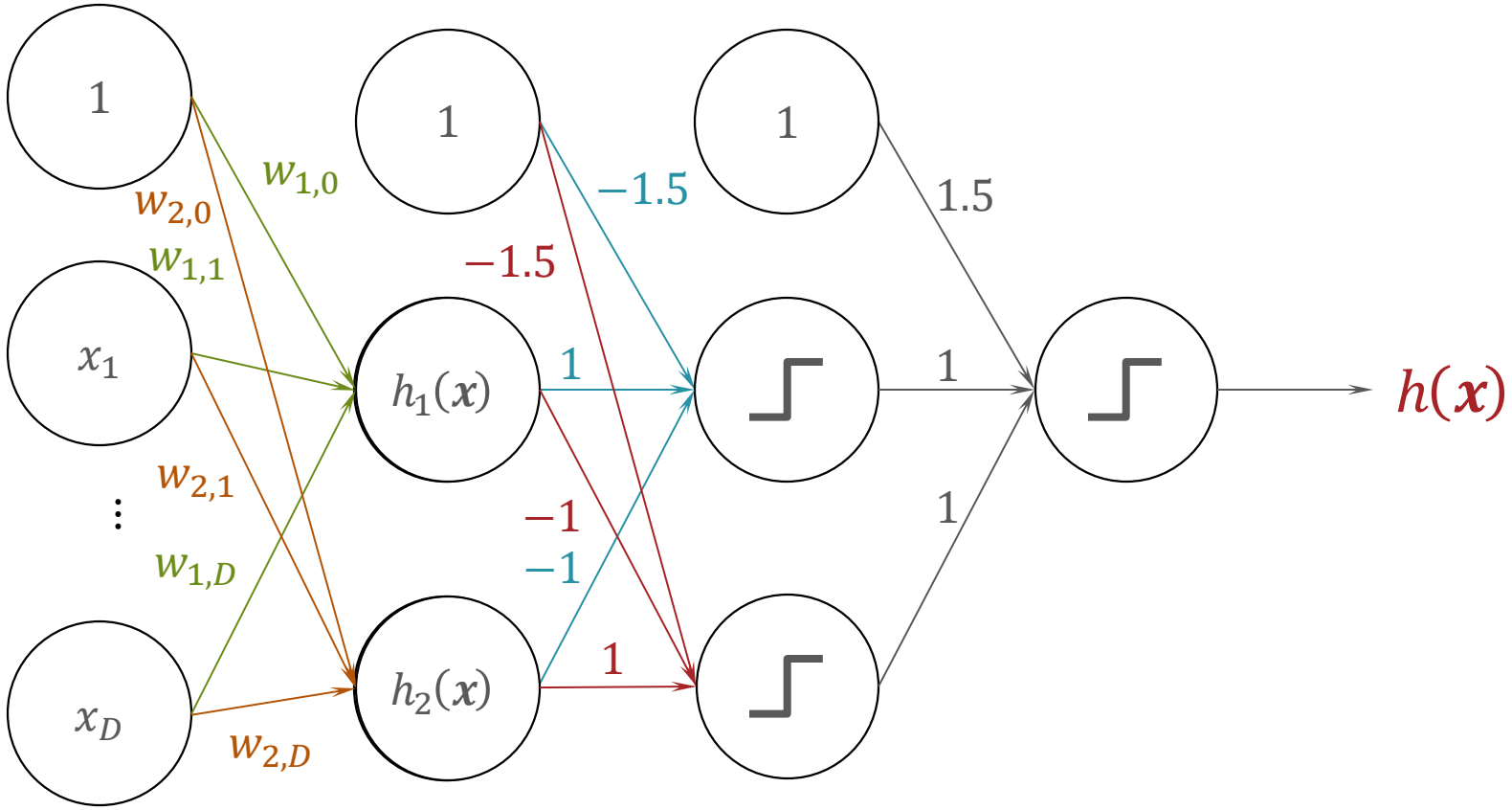
$$h(\boldsymbol{x}) = OR\left(AND\left(h_1(\boldsymbol{x}), \neg h_2(\boldsymbol{x})\right), AND\left(\neg h_1(\boldsymbol{x}), h_2(\boldsymbol{x})\right)\right)$$



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

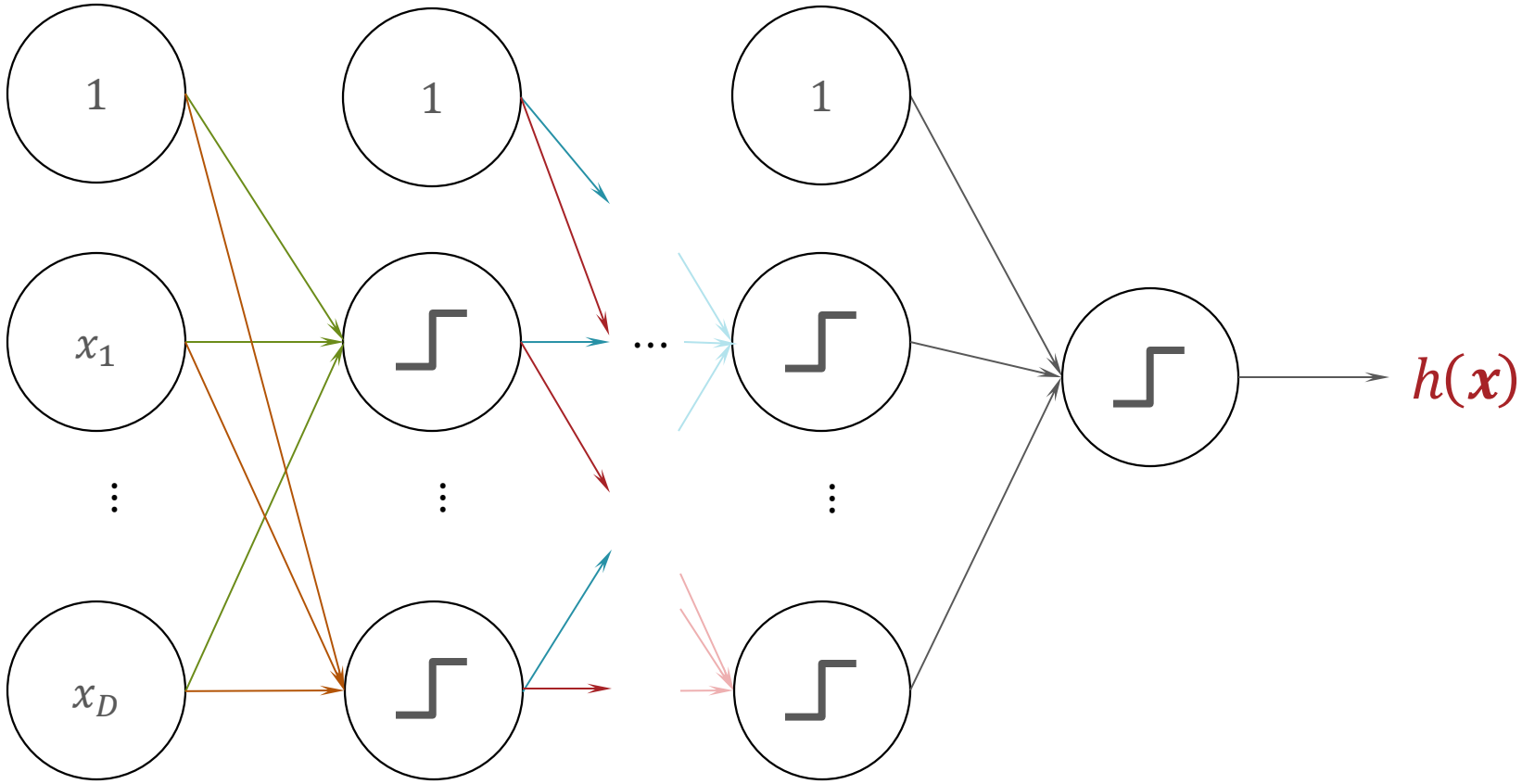
Building a Network

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

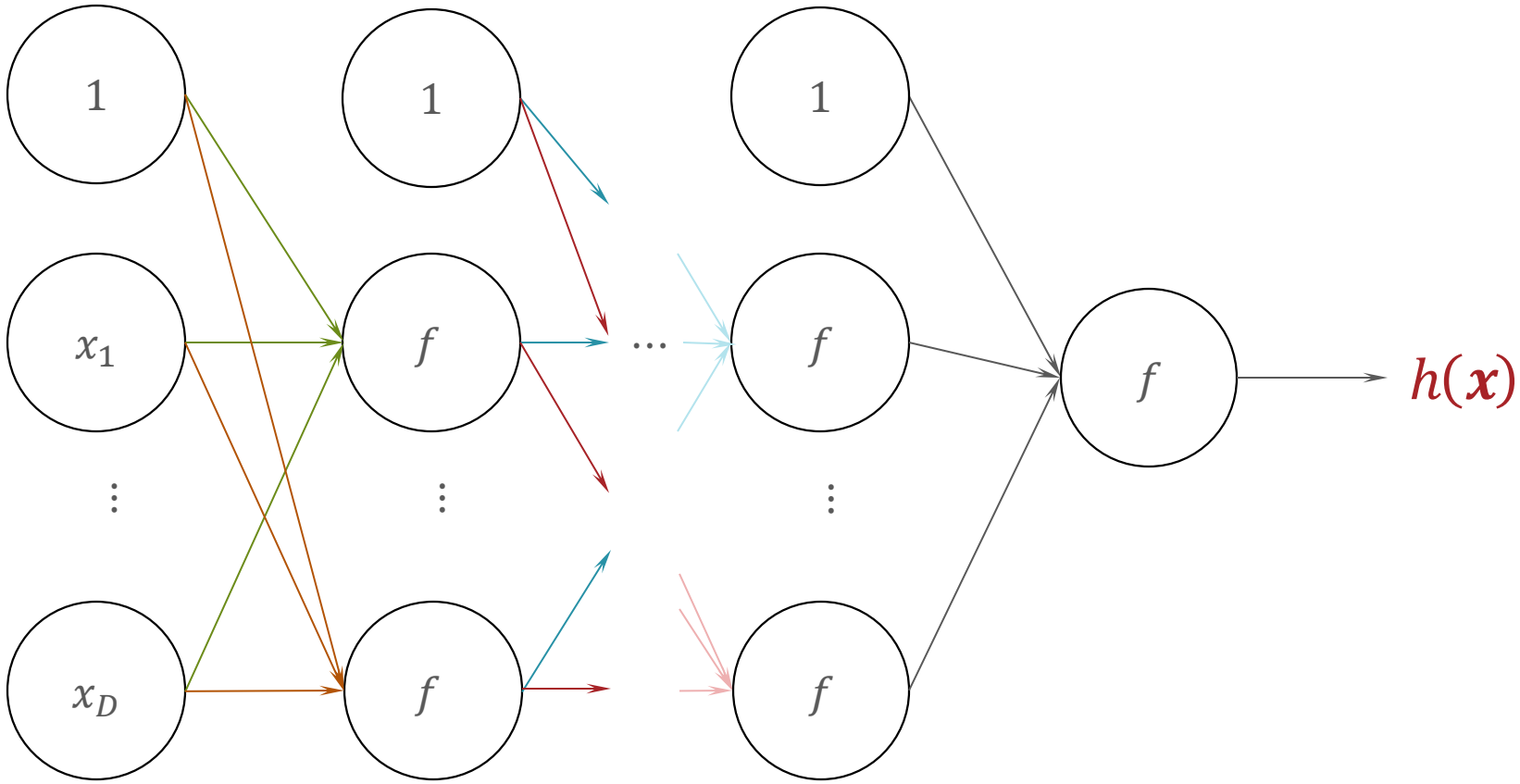


$$h(\boldsymbol{x}) = \text{sign}(\text{sign}(\text{sign}(\boldsymbol{w}_1^T\boldsymbol{x}) - \text{sign}(\boldsymbol{w}_2^T\boldsymbol{x}) - 1.5) + \text{sign}(-\text{sign}(\boldsymbol{w}_1^T\boldsymbol{x}) + \text{sign}(\boldsymbol{w}_2^T\boldsymbol{x}) - 1.5) + 1.5)$$

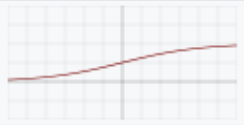
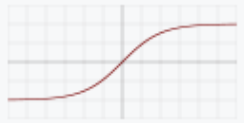
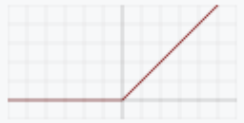
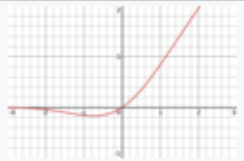
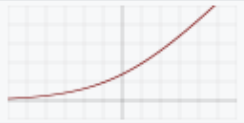
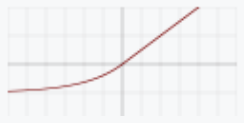
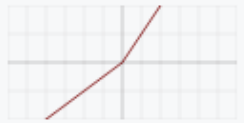
Multi-Layer Perceptron (MLP)



(Fully-Connected) Feed Forward Neural Network



Activation Functions

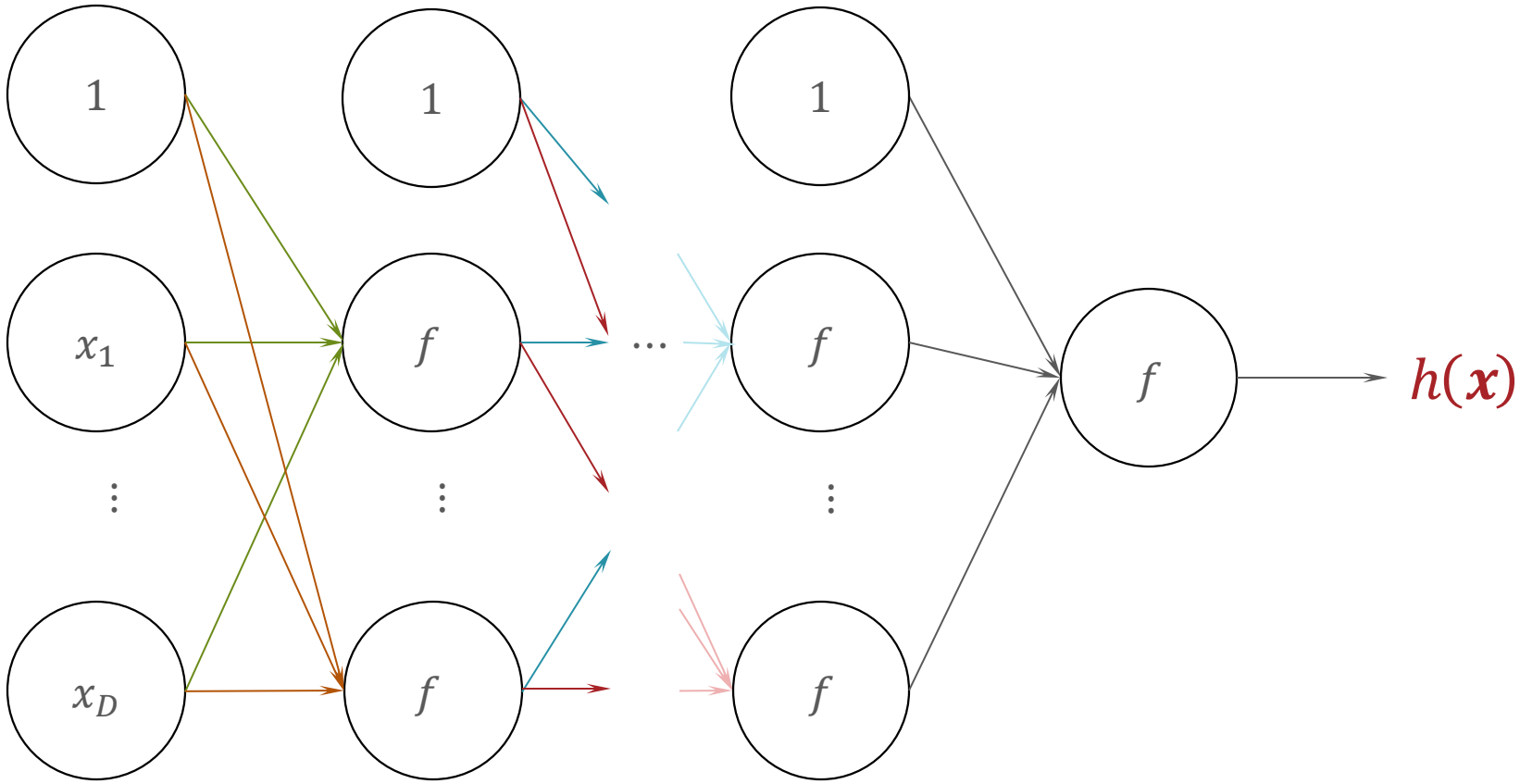
Logistic, sigmoid, or soft step		$\sigma(x) = \frac{1}{1+e^{-x}}$
Hyperbolic tangent (tanh)		$\tanh(x) = \frac{e^x - e^{-x}}{e^x + e^{-x}}$
Rectified linear unit (ReLU)[7]		$\begin{cases} 0 & \text{if } x \leq 0 \\ x & \text{if } x > 0 \end{cases}$ $= \max\{0, x\} = x\mathbf{1}_{x>0}$
Gaussian Error 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]		$\begin{cases} \alpha\left(e^x - 1\right) & \text{if } x \leq 0 \\ x & \text{if } x > 0 \end{cases}$ with parameter α
Leaky rectified linear unit (Leaky ReLU)[11]		$\begin{cases} 0.01x & \text{if } x < 0 \\ x & \text{if } x \geq 0 \end{cases}$
Parametric rectified linear unit (PReLU)[12]		$\begin{cases} \alpha x & \text{if } x < 0 \\ x & \text{if } x \geq 0 \end{cases}$ with parameter α

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

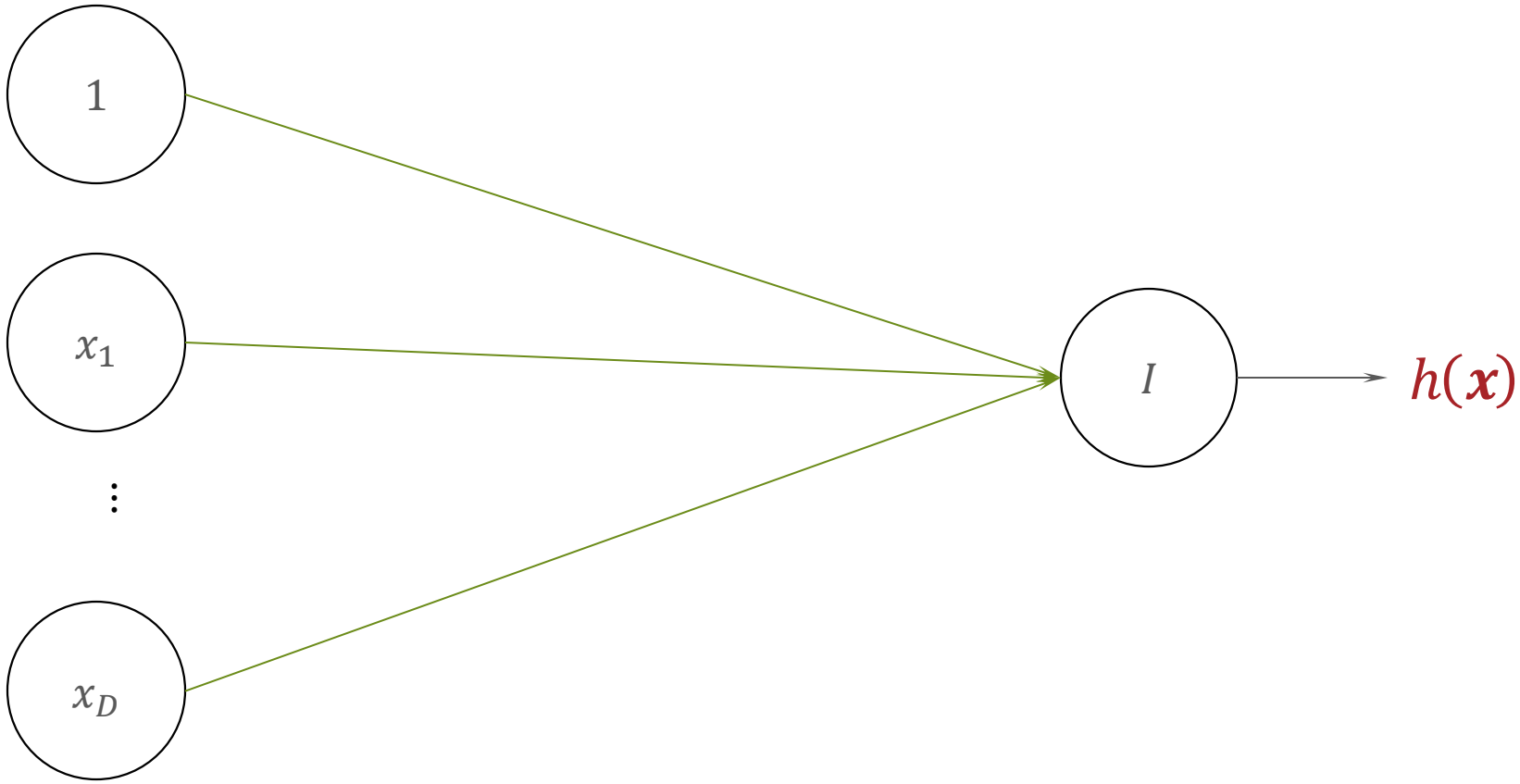
Poll Question 2

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

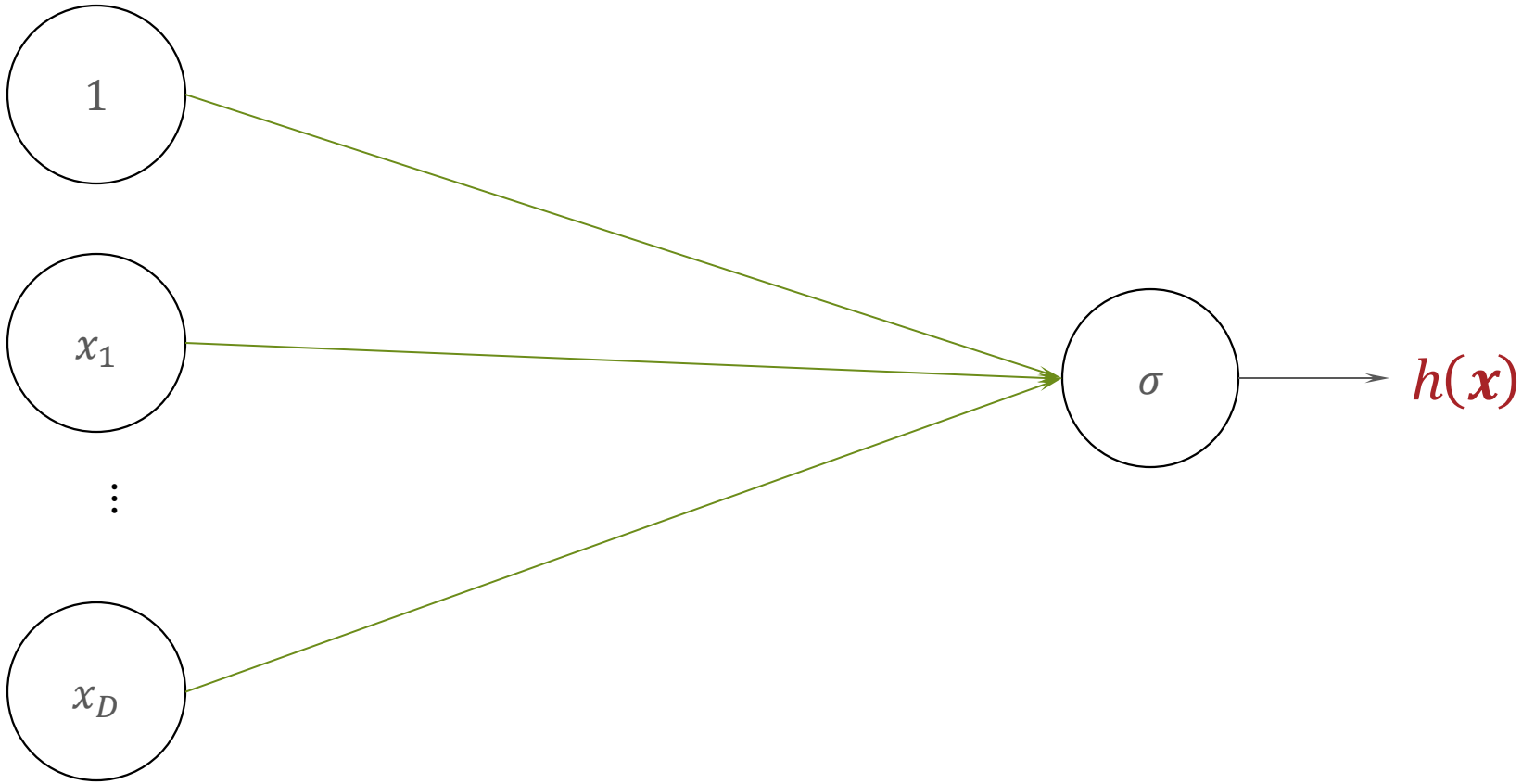
A. Only true for linear regression
B. Only true for logistic regression
C. TOXIC
D. True for both
E. False for both



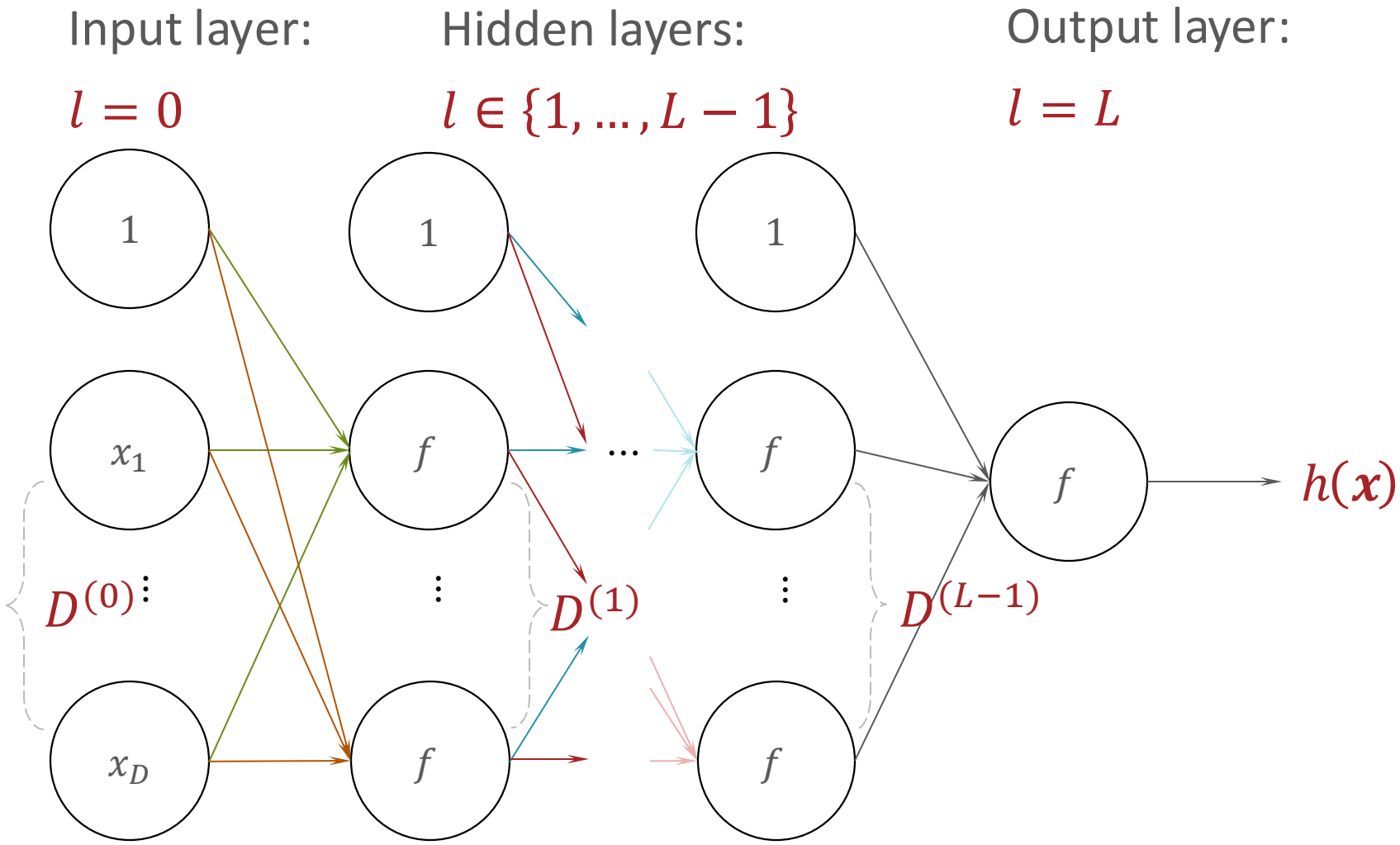
Linear Regression as a Neural Network



Logistic Regression as a Neural Network



(Fully-Connected) Feed Forward Neural Network

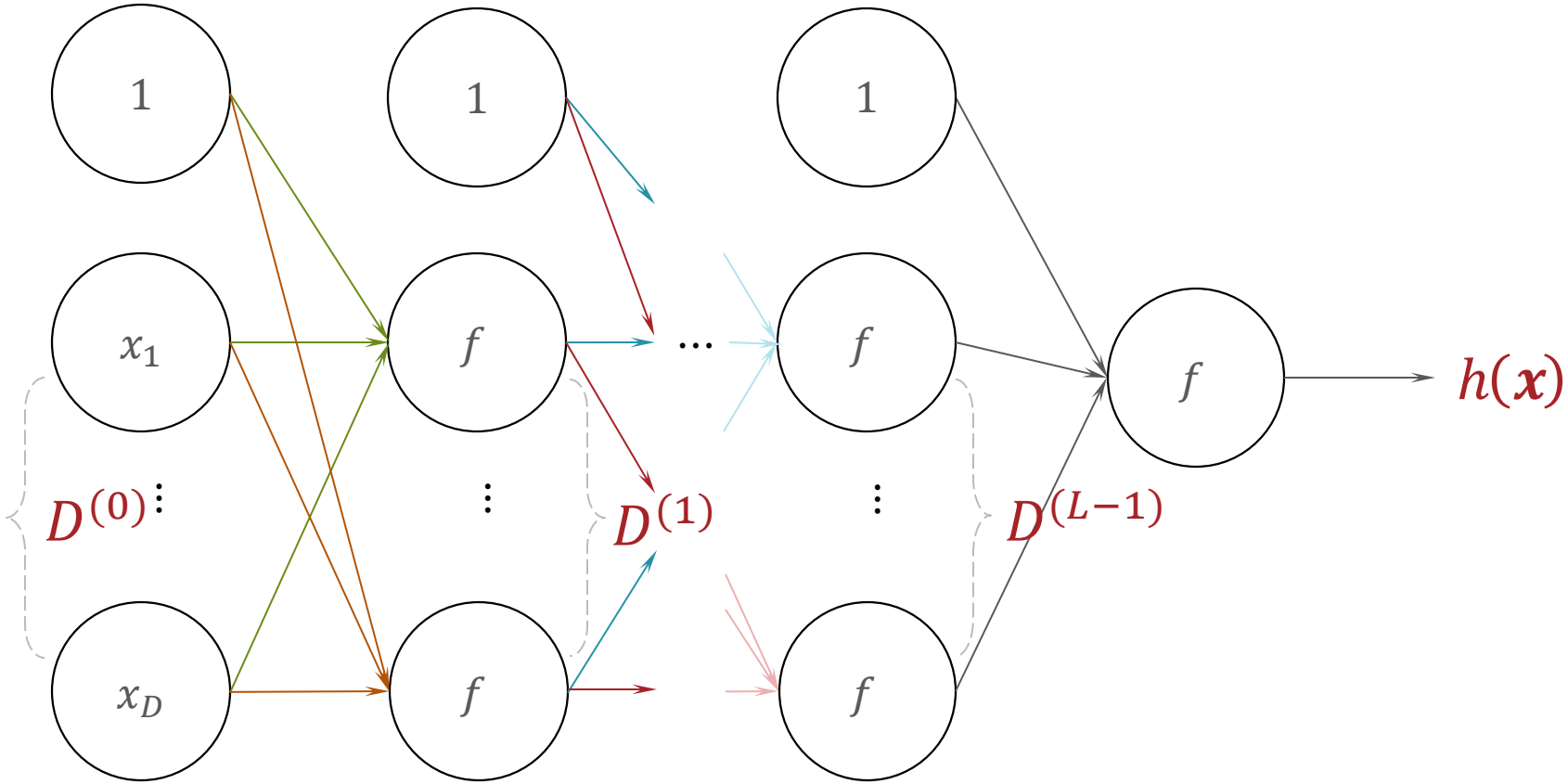


Layer l has dimension $D^{(l)}$ → Layer l has $D^{(l)} + 1$ nodes, counting the bias node

(Fully-Connected) Feed Forward Neural Network

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

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

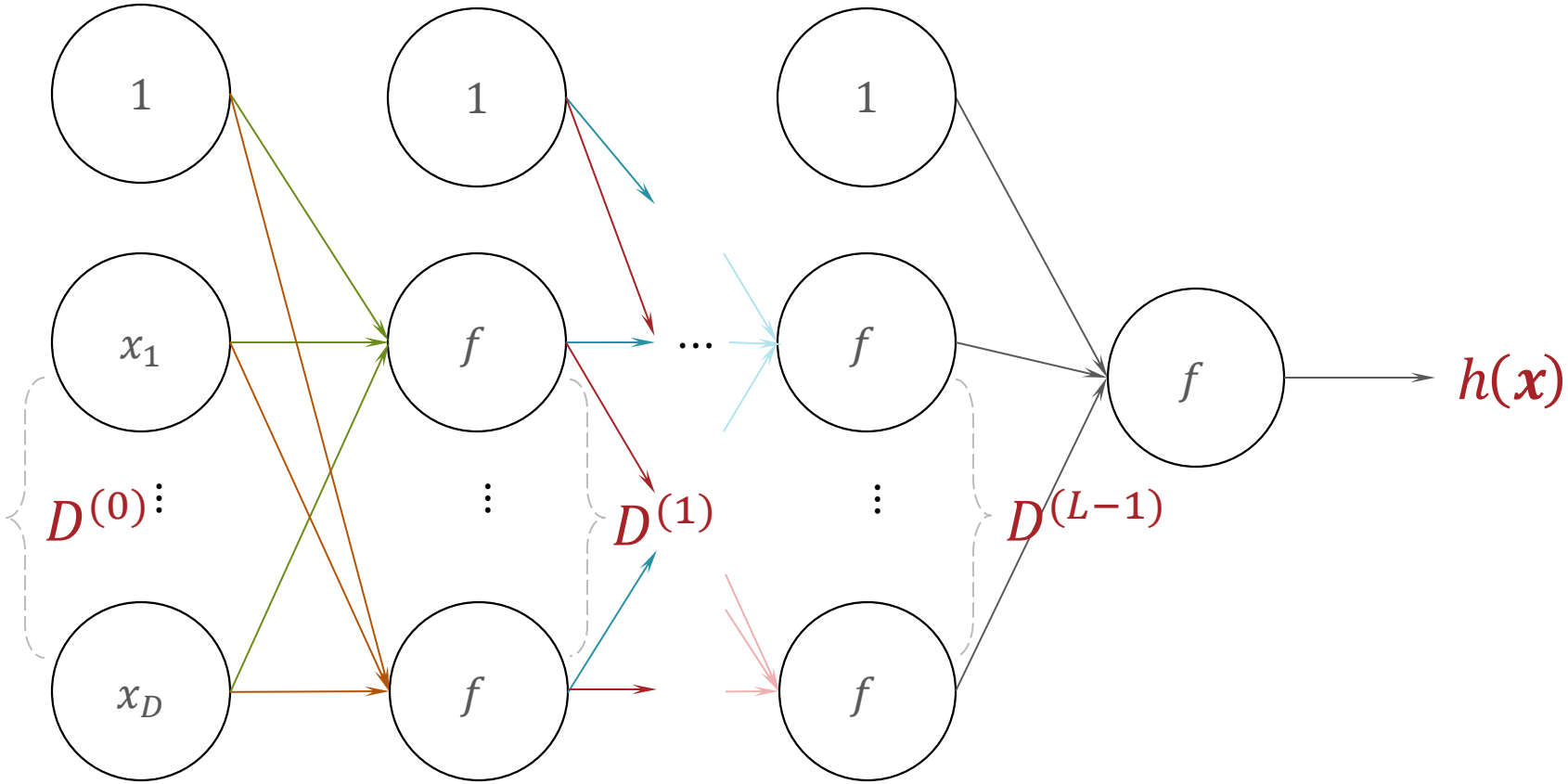


$w_{j,i}^{(l)}$ is the weight between node i in layer $l-1$ and node j in layer l

So what are all these layers doing for us anyway?

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

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



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

Neural Network Decision Boundaries: Example 1

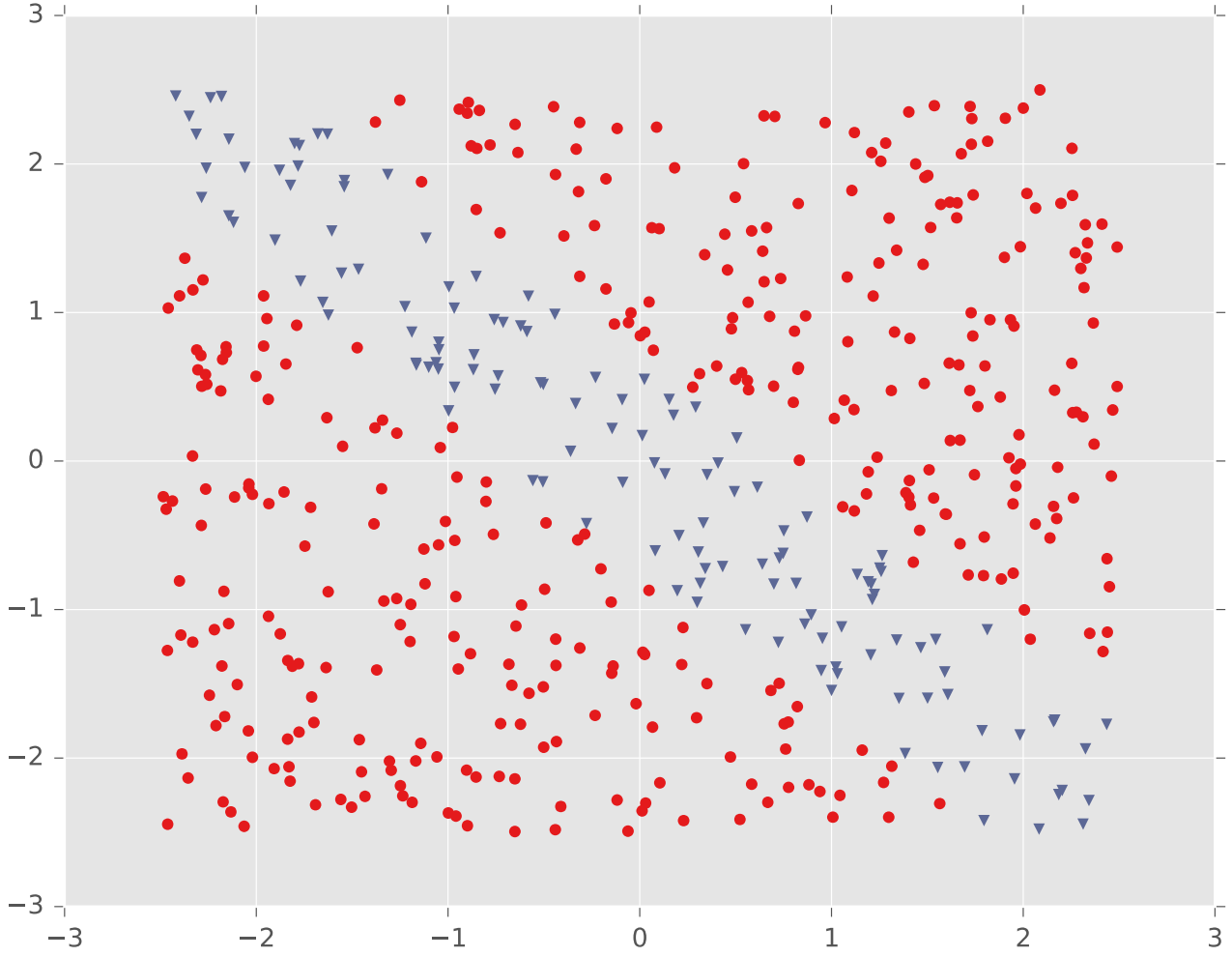


Figure courtesy of Matt Gormley

Neural Network Decision Boundaries: Example 1

Figure courtesy of Matt Gormley

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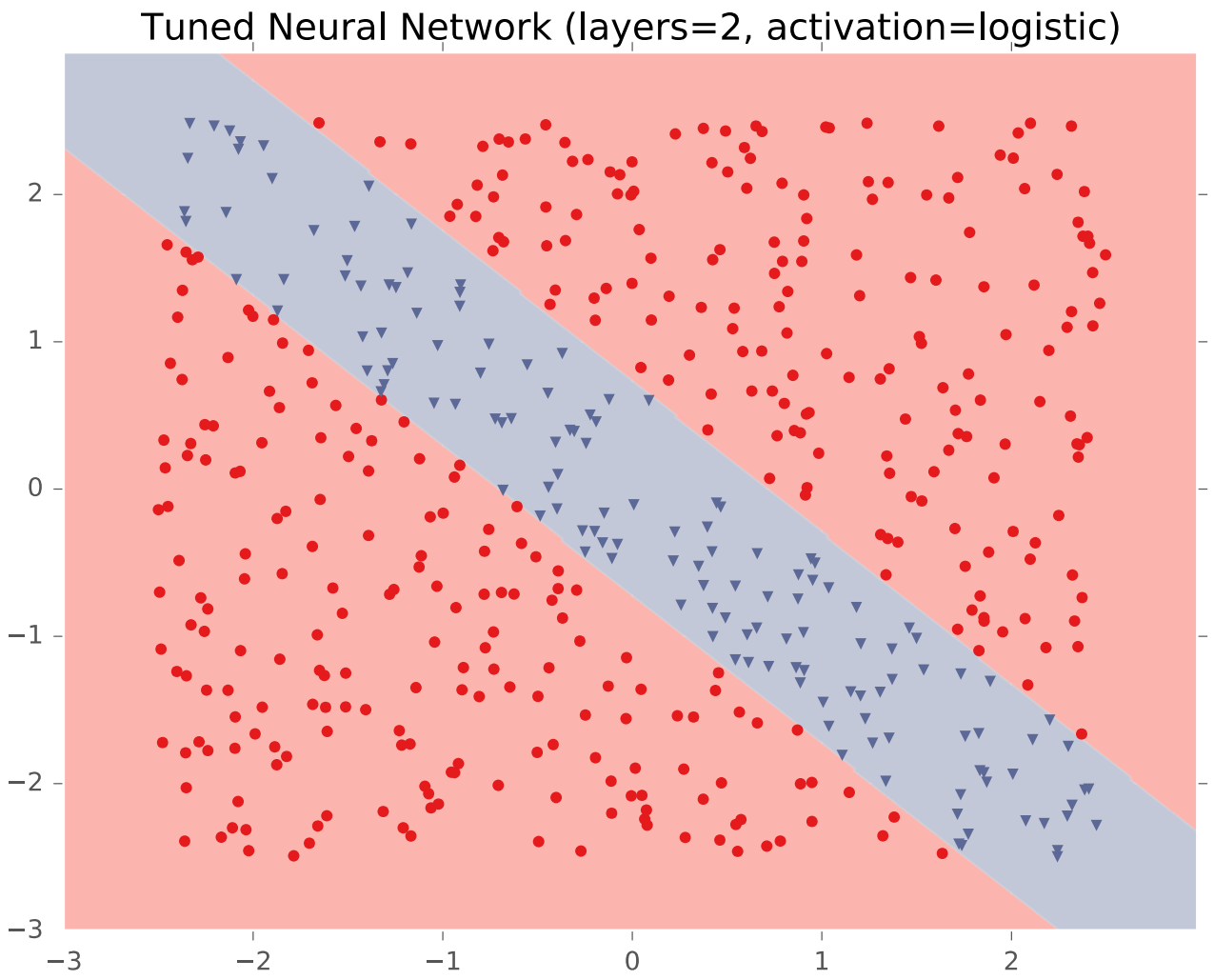

Figure courtesy of Matt Gormley

Neural Network Decision Boundaries: Example 1

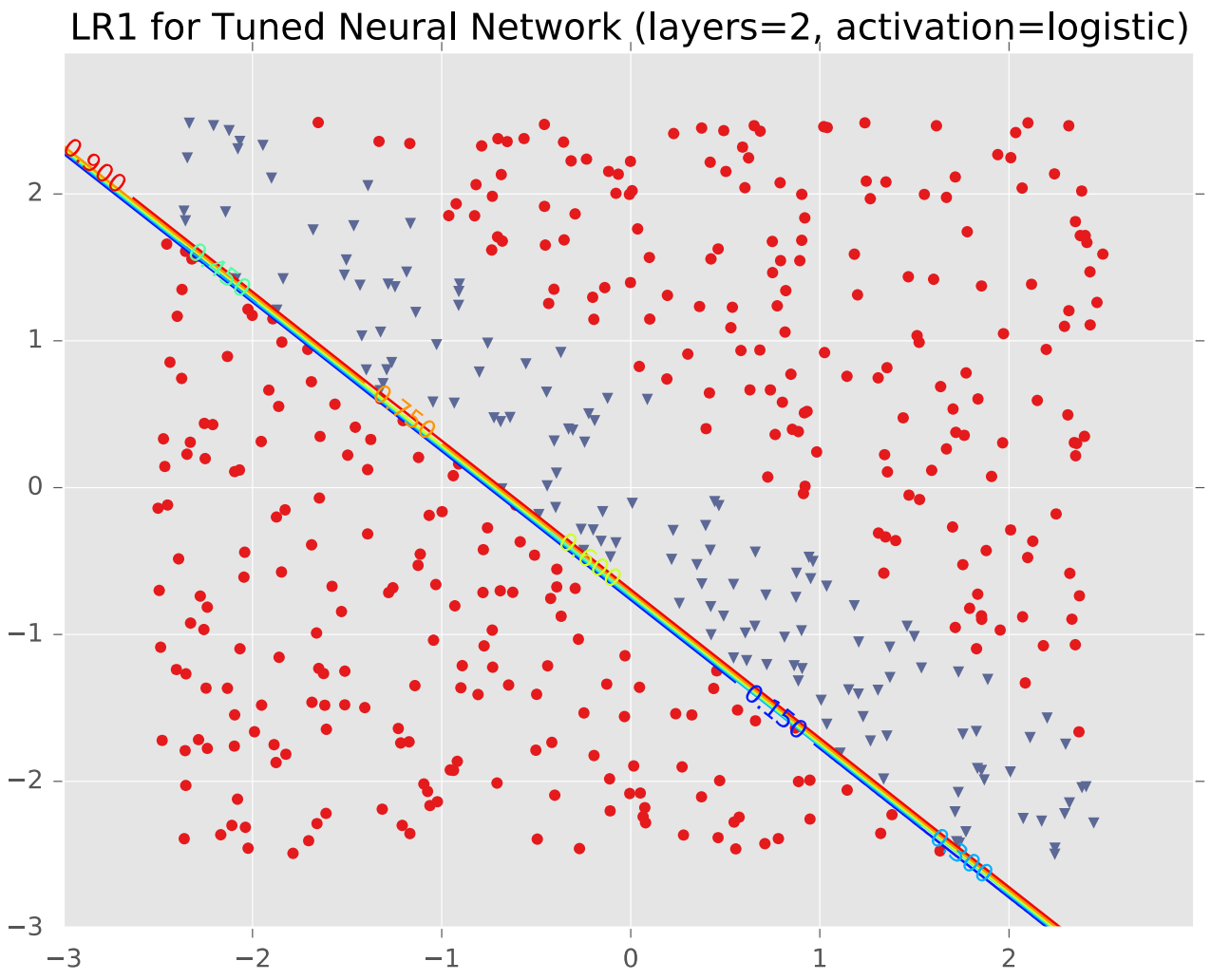

Figure courtesy of Matt Gormley

Neural Network Decision Boundaries: Example 1

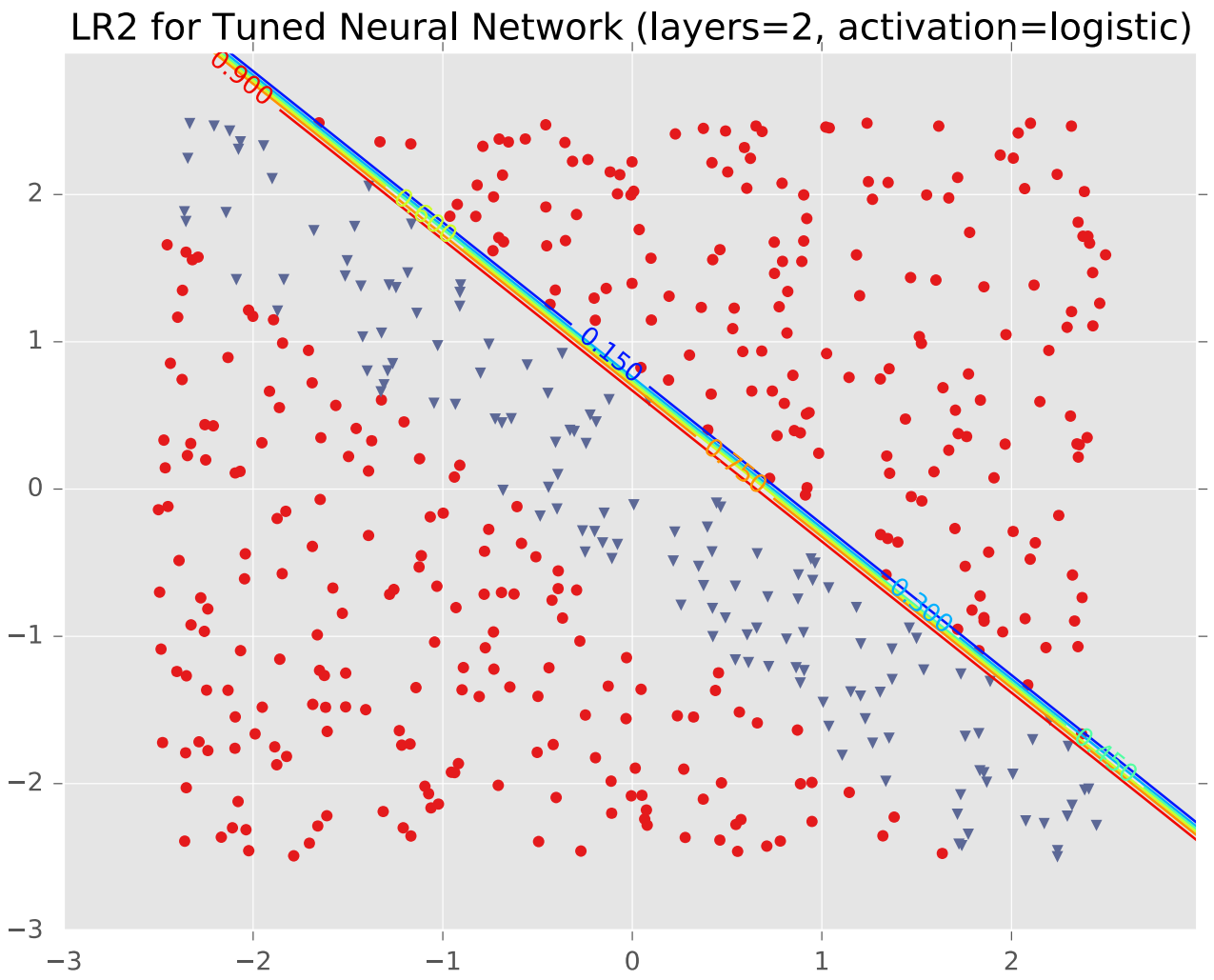

Figure courtesy of Matt Gormley

Neural Network Decision Boundaries: Example 1

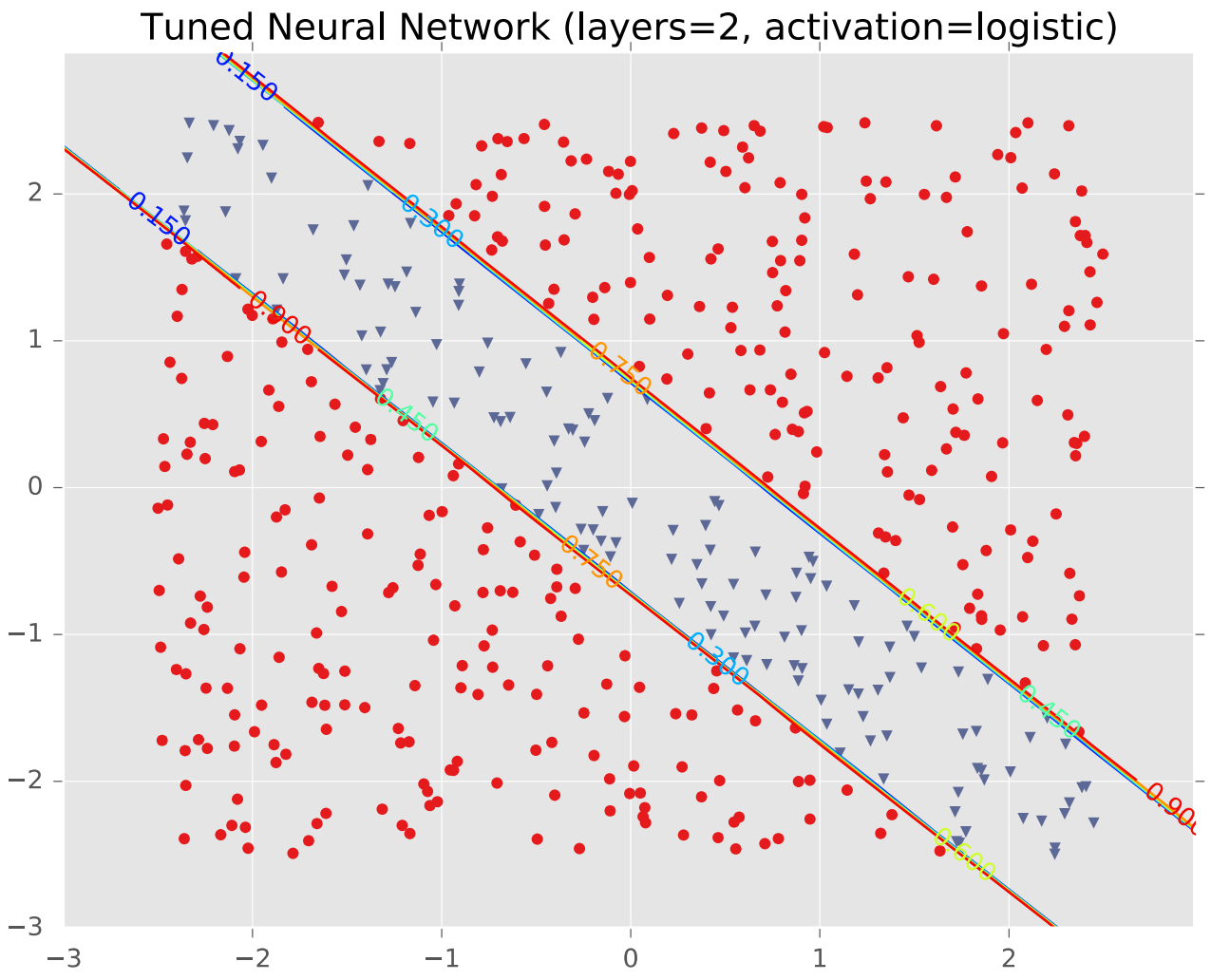

Figure courtesy of Matt Gormley

Neural Network Decision Boundaries: Example 1

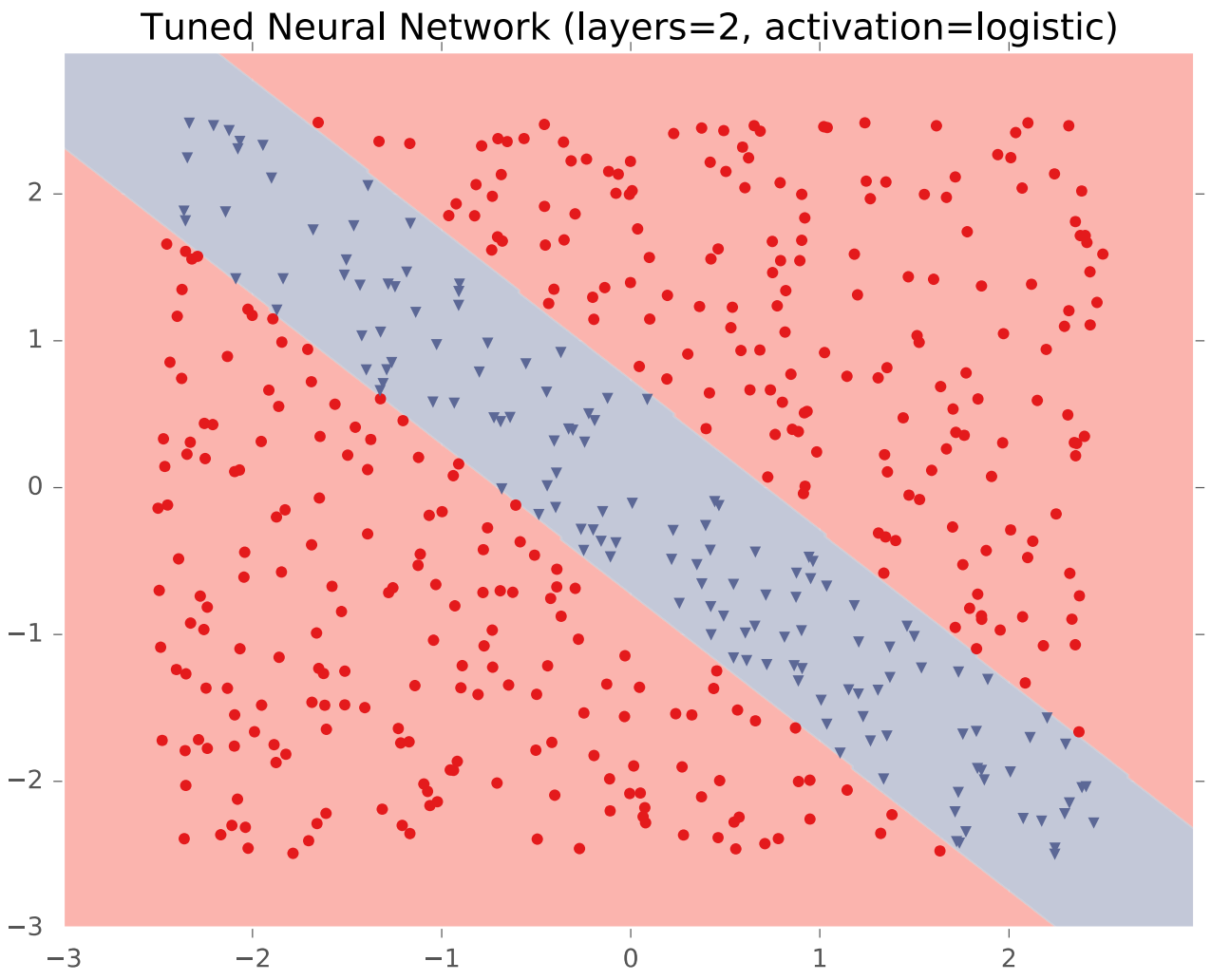

Figure courtesy of Matt Gormley

Neural Network Decision Boundaries: Example 2

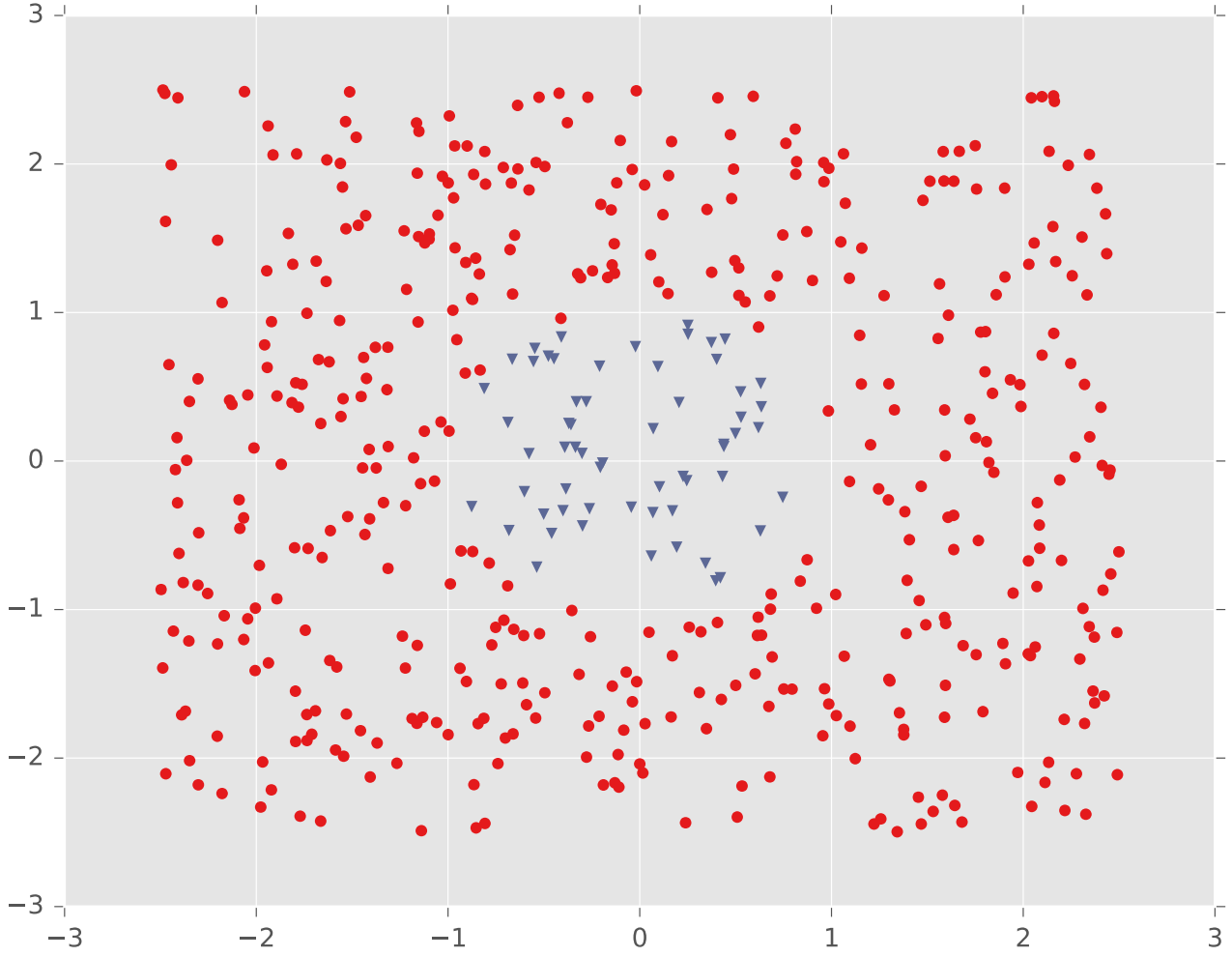

Figure courtesy of Matt Gormley

Neural Network Decision Boundaries: Example 2

Figure courtesy of Matt Gormley

Neural Network Decision Boundaries: Example 2

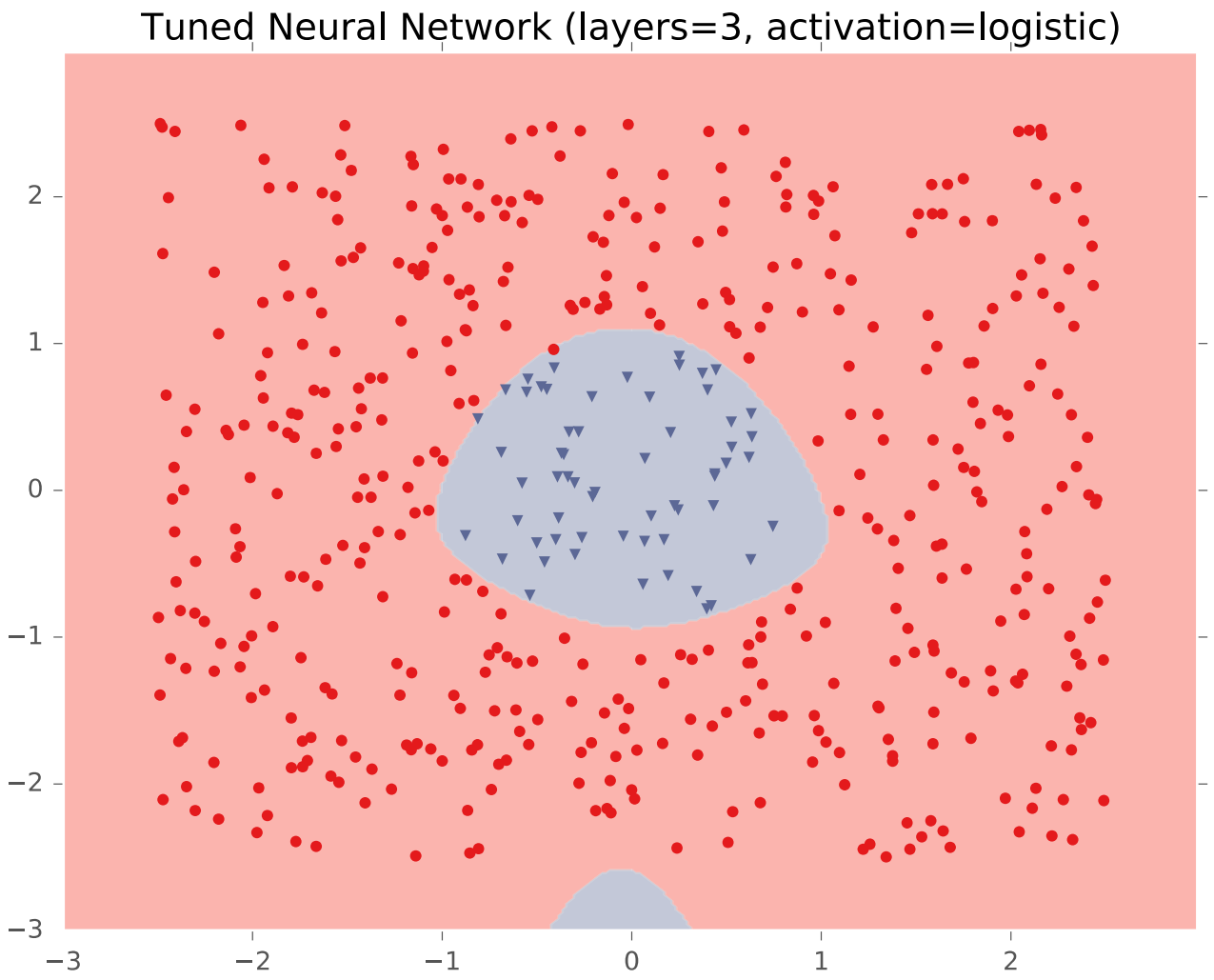

Figure courtesy of Matt Gormley

Neural Network Decision Boundaries: Example 2

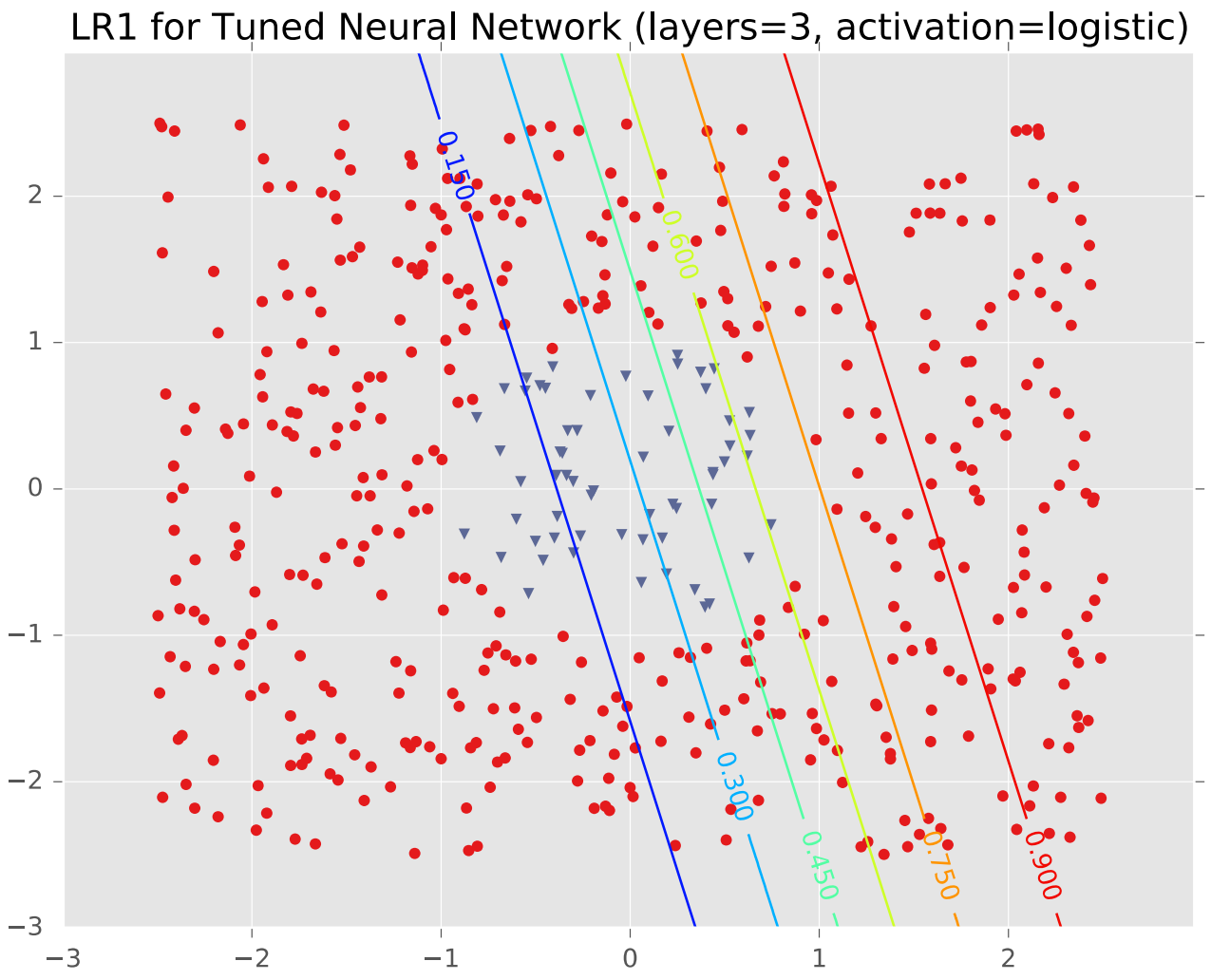

Figure courtesy of Matt Gormley

Neural Network Decision Boundaries: Example 2

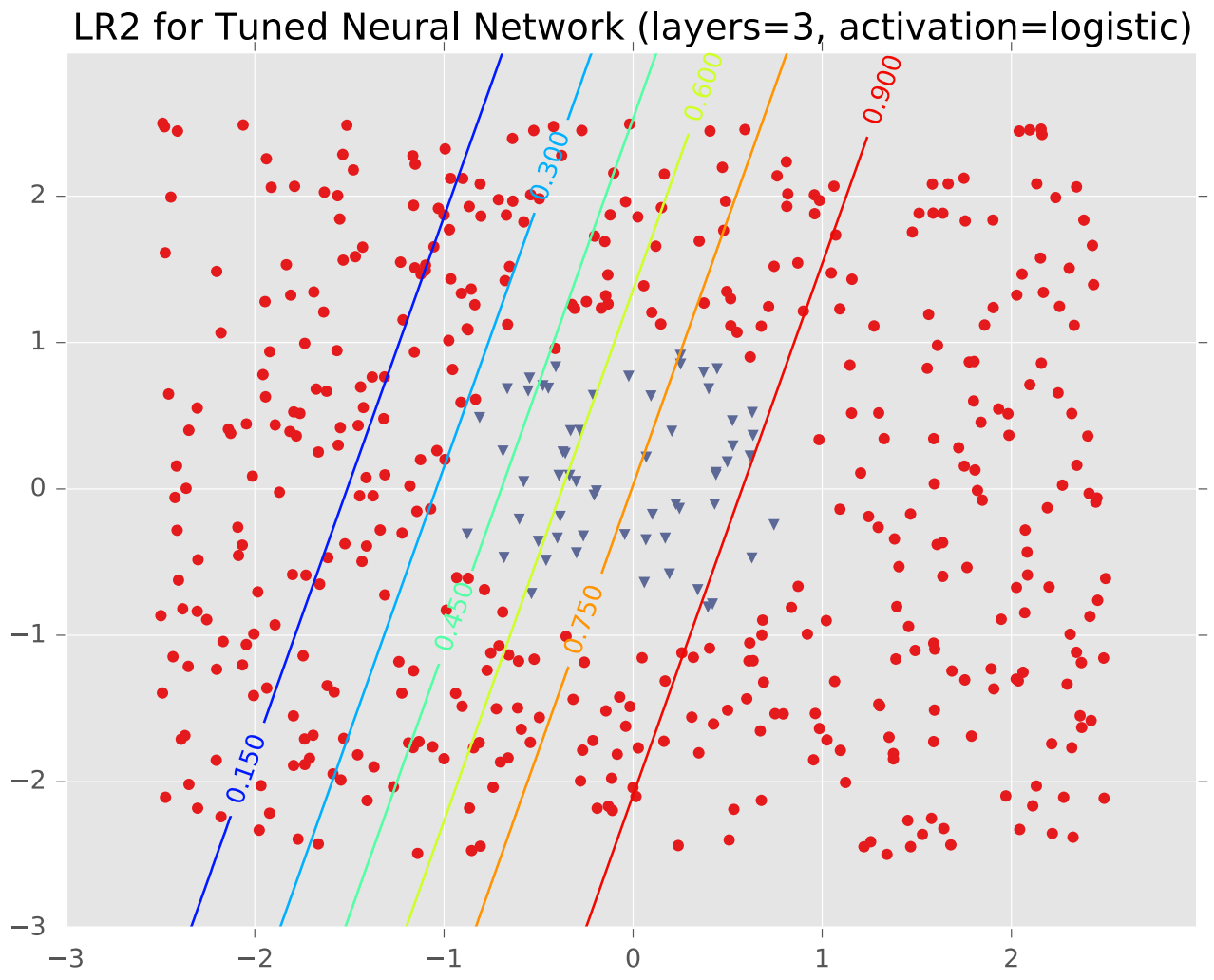

Figure courtesy of Matt Gormley

Neural Network Decision Boundaries: Example 2

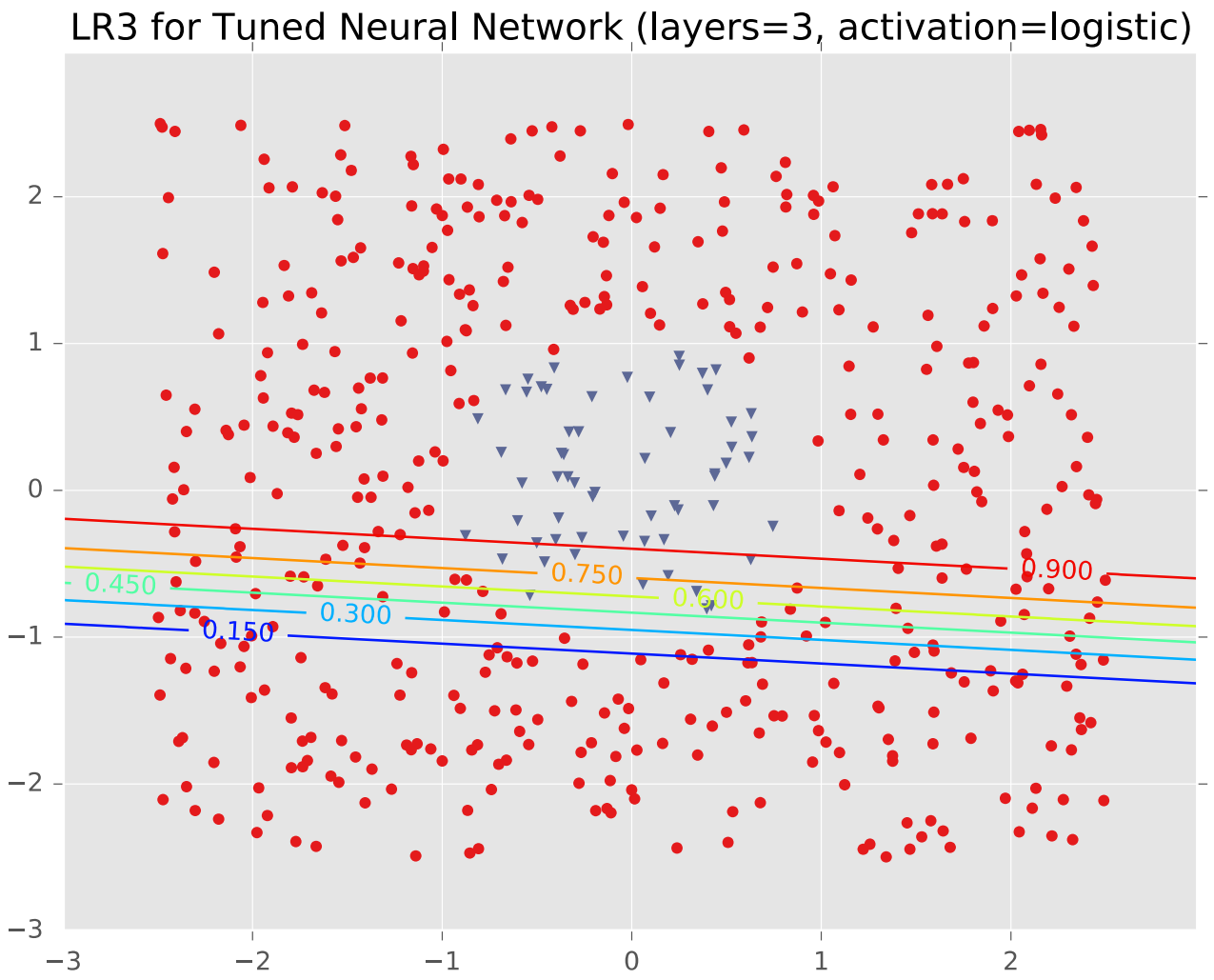

Figure courtesy of Matt Gormley

Neural Network Decision Boundaries: Example 2

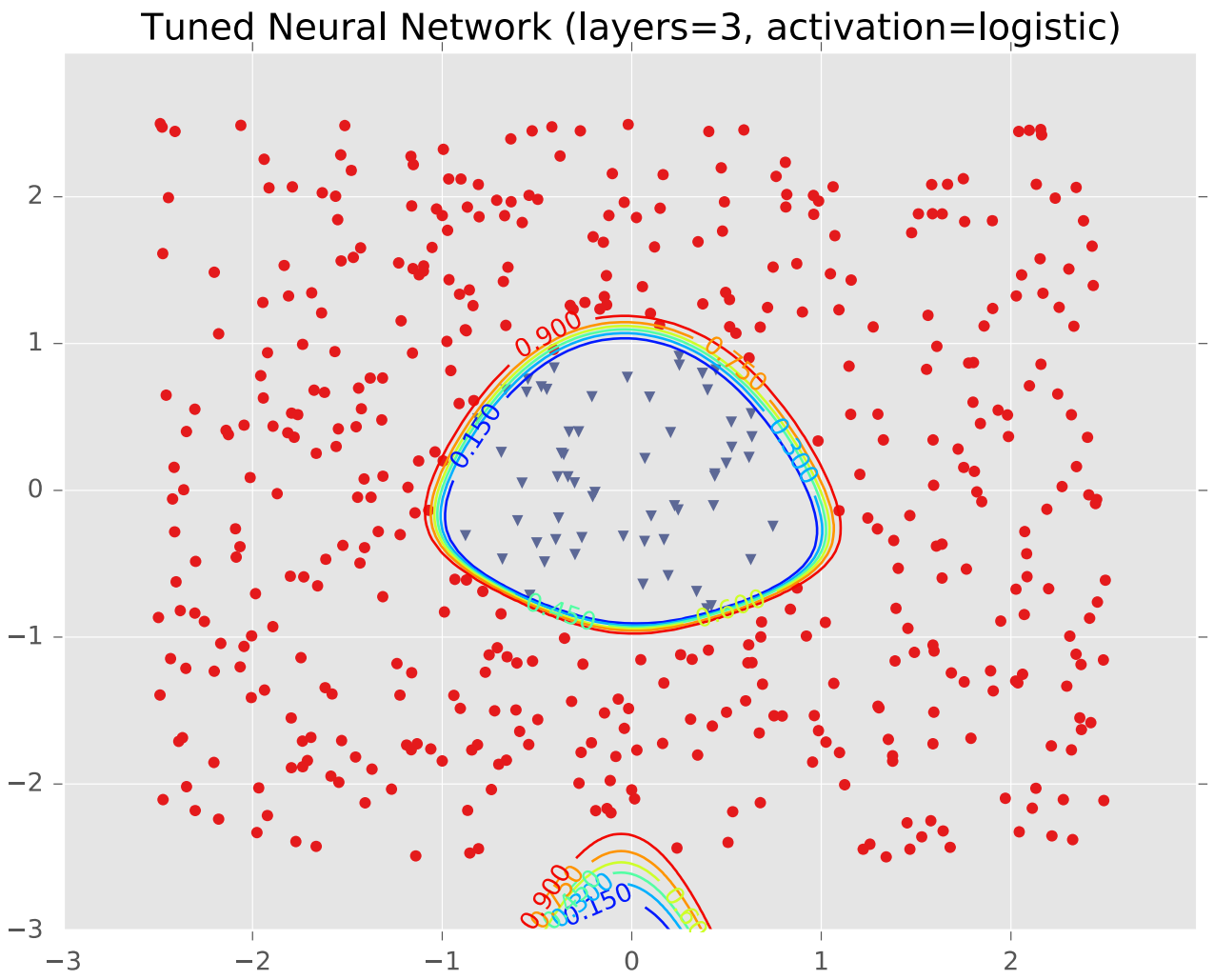

Figure courtesy of Matt Gormley

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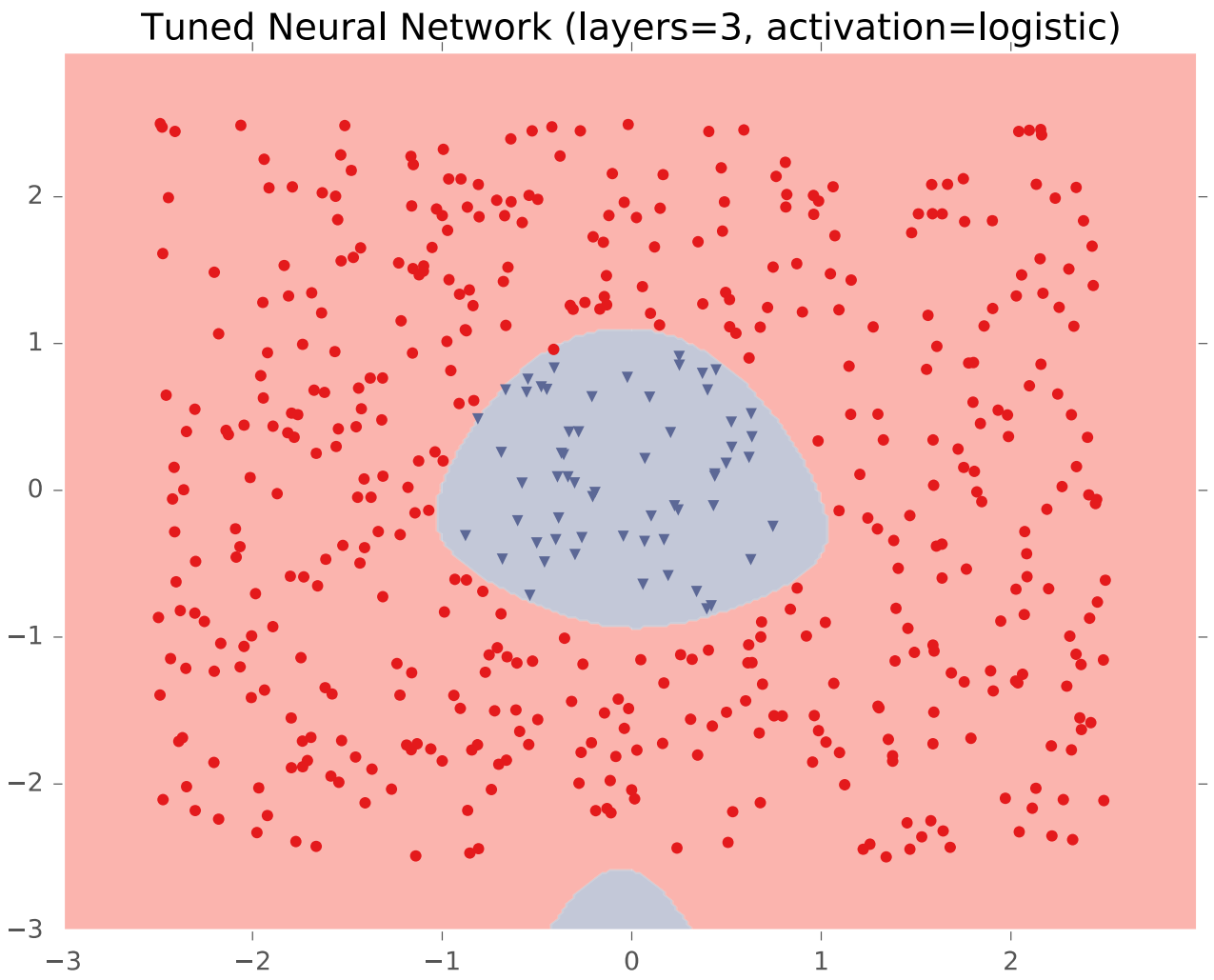
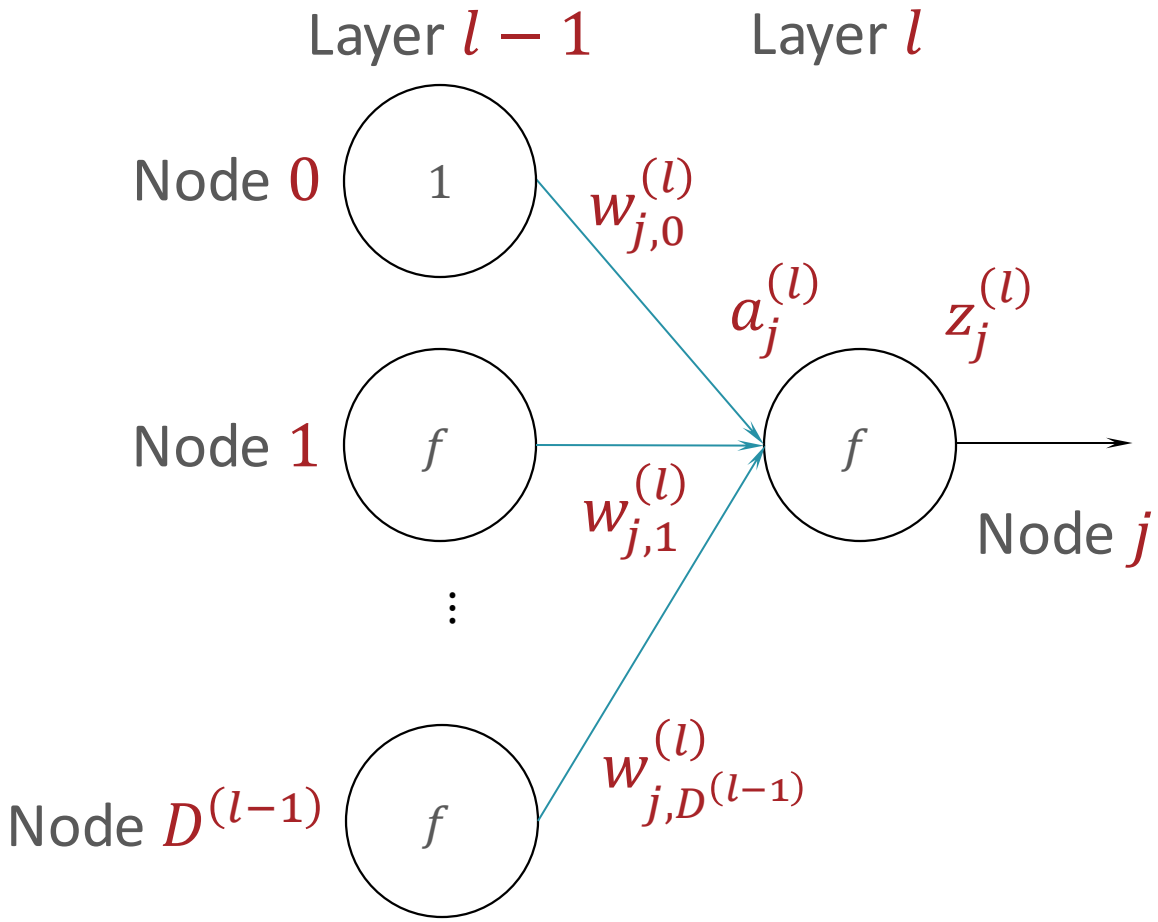


Figure courtesy of Matt Gormley

Signal and Outputs

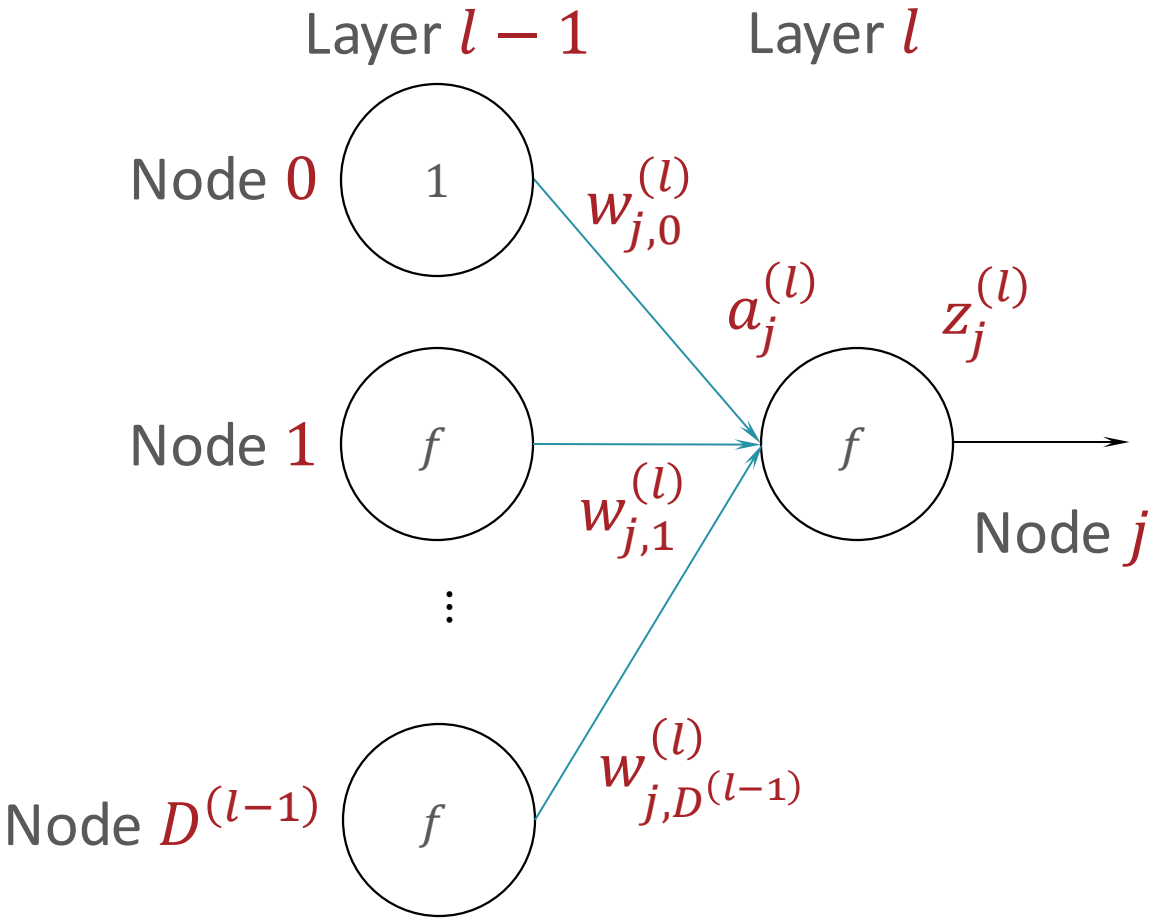
Every node has an incoming *signal* and outgoing *output*



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

Signal and Outputs

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



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

Forward Propagation for Making Predictions

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

Okay, but where do these weights $W^{(1)}, \dots, W^{(L)}$ come from?

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

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