Machine Learning Department
School of Computer Science
Carnegie Mellon University

Neural Networks

Matt Gormley
Lecture 11
Feb. 23, 2022

Reminders

- Post-Exam Followup:
  - Exam Viewing
  - Exit Poll: Exam 1
  - Grade Summary 1
- Homework 4: Logistic Regression
  - Out: Fri, Feb 18
  - Due: Sun, Feb. 27 at 11:59pm
- Swapped lecture/recitation:
  - Lecture 12: Fri, Feb. 25

OPTIMIZATION FOR L1 REGULARIZATION

Optimization for L1 Regularization

Can we apply SGD to the LASSO learning problem?

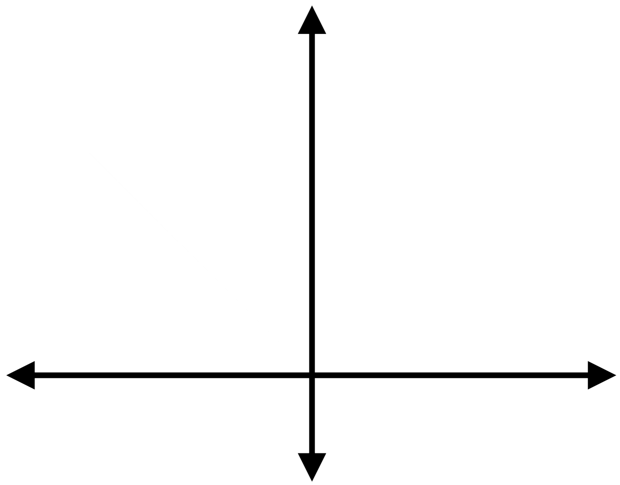
$$\underset{\boldsymbol{\theta}}{\text{argmin}} \;\; J_{\text{LASSO}}(\boldsymbol{\theta})$$

$$\begin{aligned} J_{\text{LASSO}}(\boldsymbol{\theta}) &= J(\boldsymbol{\theta}) + \boxed{\lambda ||\boldsymbol{\theta}||_1} \\ &= \frac{1}{2}\sum_{i=1}^{N}(\boldsymbol{\theta}^T\mathbf{x}^{(i)} - y^{(i)})^2 + \boxed{\lambda \sum_{k=1}^{K} |\theta_k|} \end{aligned}$$

Optimization for L1 Regularization

- Consider the absolute value function:

$$r(\boldsymbol{\theta}) = \lambda \sum_{k=1}^{K} |\theta_k|$$



- The L1 penalty is subdifferentiable (i.e. not differentiable at 0)

Def: A vector $g \in \mathbb{R}^M$ is called a **subgradient** of a function $f(\mathbf{x}) : \mathbb{R}^M \rightarrow \mathbb{R}$ at the point $\mathbf{x}$ if, for all $\mathbf{x}' \in \mathbb{R}^M$, we have:

$$f(\mathbf{x}') \geq f(\mathbf{x}) + \mathbf{g}^T(\mathbf{x}' - \mathbf{x})$$

Optimization for L1 Regularization

- The L1 penalty is subdifferentiable (i.e. not differentiable at 0)
- An array of optimization algorithms exist to handle this issue:
  – Subgradient descent
  – Stochastic subgradient descent
  – Coordinate Descent
  – Othant-Wise Limited memory Quasi-Newton (OWL-QN) (Andrew & Gao, 2007) and provably convergent variants
  – Block coordinate Descent (Tseng & Yun, 2009)
  – Sparse Reconstruction by Separable Approximation (SpaRSA) (Wright et al., 2009)
  – Fast Iterative Shrinkage Thresholding Algorithm (FISTA) (Beck & Teboulle, 2009)

Basically the same as GD and SGD, but you use one of the subgradients when necessary

NEURAL NETWORKS

Background

A Recipe for Machine Learning

1. Given training data:

$$\{\boldsymbol{x}_i, \boldsymbol{y}_i\}_{i=1}^N$$

Face *Face* *Not a face*

2. Choose each of these:
   – Decision function

$$\hat{\boldsymbol{y}} = f_{\boldsymbol{\theta}}(\boldsymbol{x}_i)$$

Examples: Linear regression, Logistic regression, Neural Network

   – Loss function

$$\ell(\hat{\boldsymbol{y}}, \boldsymbol{y}_i) \in \mathbb{R}$$

Examples: Mean-squared error, Cross Entropy

Background

A Recipe for Machine Learning

1. Given training data:

$$\{\boldsymbol{x}_i, \boldsymbol{y}_i\}_{i=1}^N$$

2. Choose each of these:
   - Decision function

$$\hat{\boldsymbol{y}} = f_{\boldsymbol{\theta}}(\boldsymbol{x}_i)$$

   - Loss function

$$\ell(\hat{\boldsymbol{y}}, \boldsymbol{y}_i) \in \mathbb{R}$$

3. Define goal:

$$\boldsymbol{\theta}^* = \arg\min_{\boldsymbol{\theta}} \sum_{i=1}^N \ell(f_{\boldsymbol{\theta}}(\boldsymbol{x}_i), \boldsymbol{y}_i)$$

4. Train with SGD:
(take small steps opposite the gradient)

$$\boldsymbol{\theta}^{(t+1)} = \boldsymbol{\theta}^{(t)} - \eta_t \nabla \ell(f_{\boldsymbol{\theta}}(\boldsymbol{x}_i), \boldsymbol{y}_i)$$

Background

A Recipe for

Gradients

Backpropagation can compute this gradient!

And it's a **special case of a more general algorithm** called reverse-mode automatic differentiation that can compute the gradient of any differentiable function efficiently!

1. Given training dat

$$\{\boldsymbol{x}_i, \boldsymbol{y}_i\}_{i=1}^N$$

2. Choose each of th

– Decision functio

$$\hat{y} = f_{\boldsymbol{\theta}}(\boldsymbol{x}_i)$$

– Loss function

$$\ell(\hat{\boldsymbol{y}}, \boldsymbol{y}_i) \in \mathbb{R}$$

opp site the gradient)

$$\boldsymbol{\theta}^{(t} \quad (t) - \eta_t \nabla \ell(f_{\boldsymbol{\theta}}(\boldsymbol{x}_i), \boldsymbol{y}_i)$$

Goals for Today's Lecture

1. Explore a **new class of decision functions** (Neural Networks)
2. Consider **variants of this recipe** for training

A Recipe for

2. Choose each of these:
   – Decision function

$$\hat{y} = f_{\boldsymbol{\theta}}(\boldsymbol{x}_i)$$

   – Loss function

$$\ell(\hat{\boldsymbol{y}}, \boldsymbol{y}_i) \in \mathbb{R}$$

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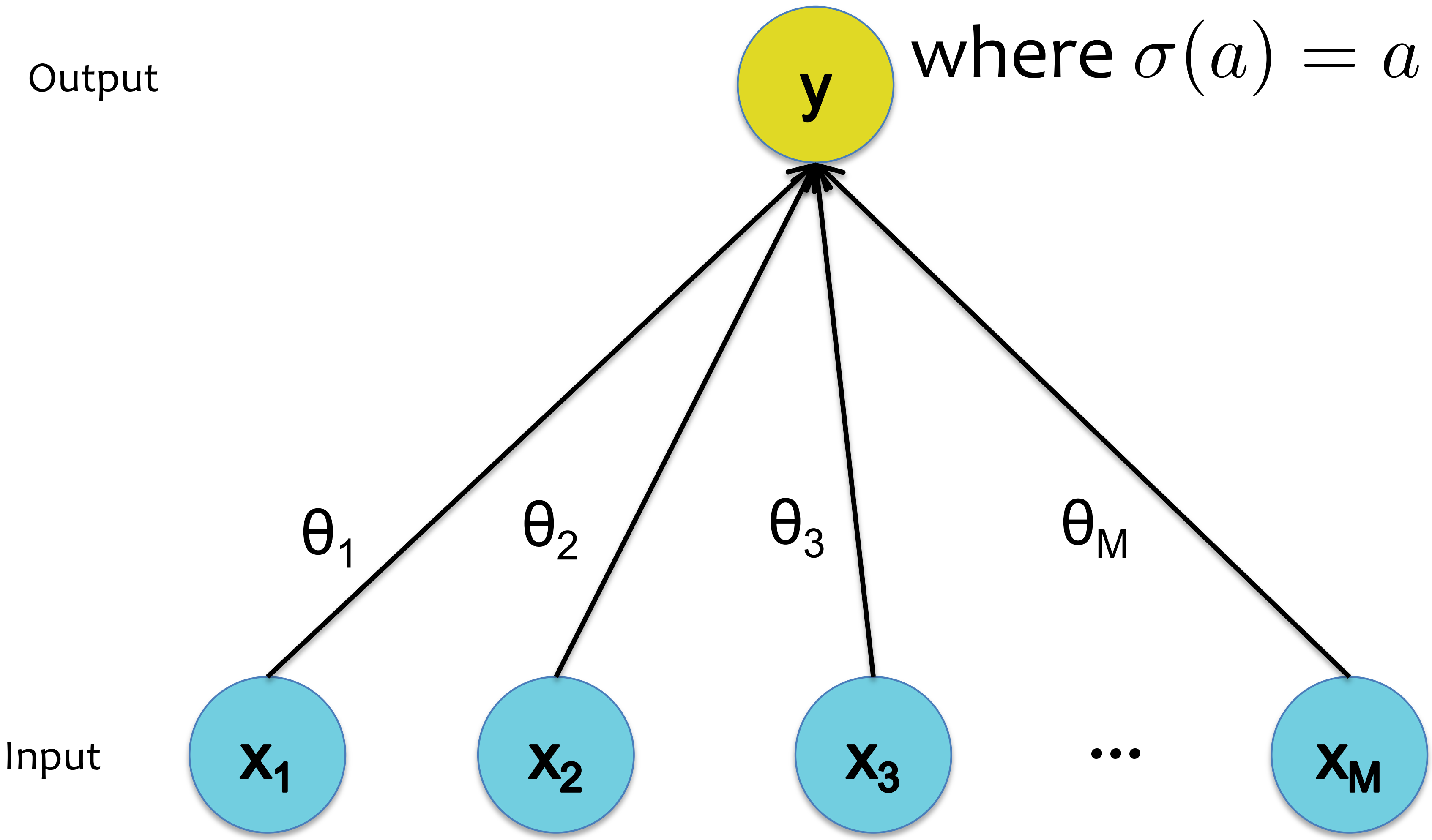
Decision Functions

Linear Regression

$$y = h_{\boldsymbol{\theta}}(\boldsymbol{x}) = \sigma(\boldsymbol{\theta}^T \boldsymbol{x})$$

where $\sigma(a) = a$

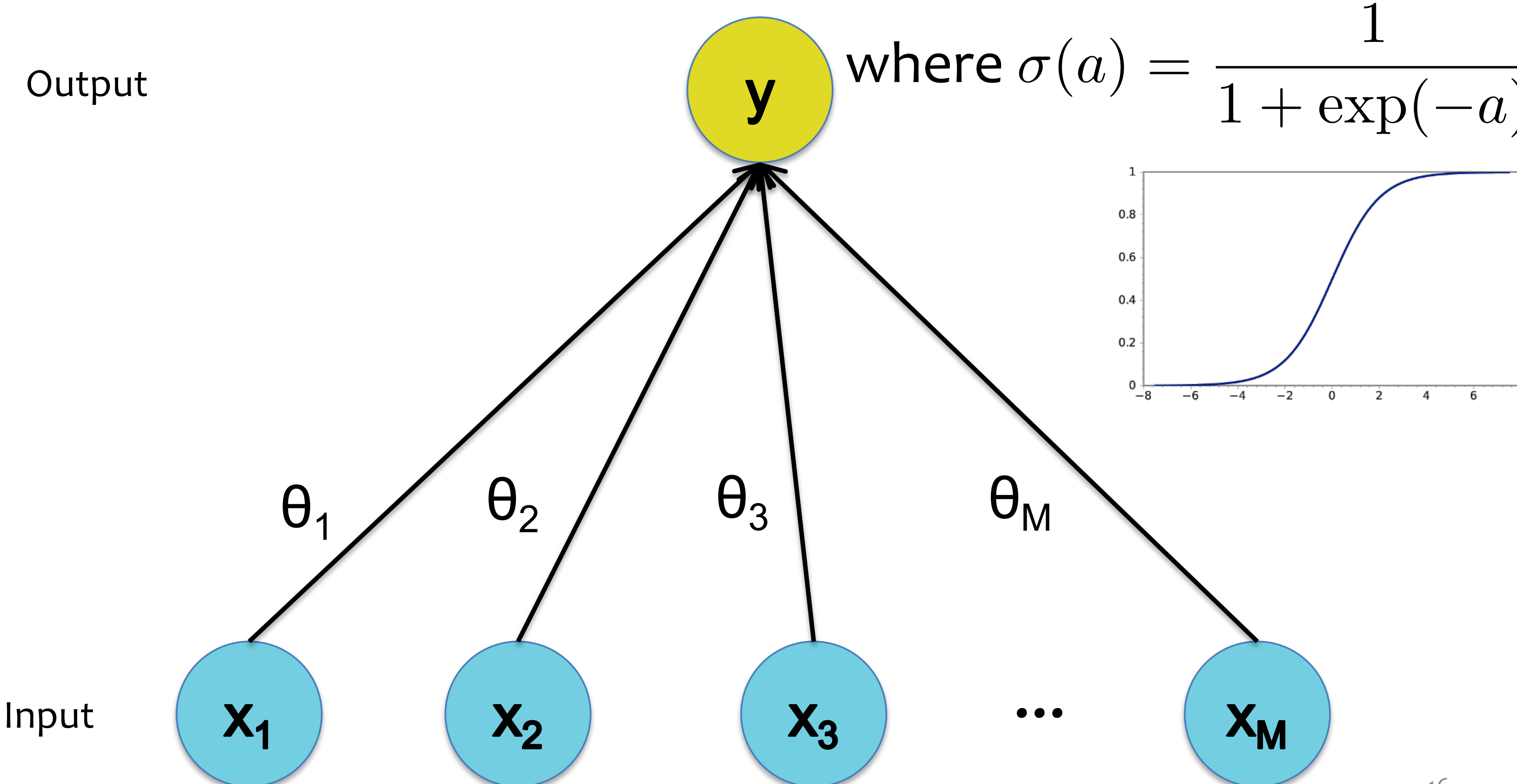


Decision Functions

Logistic Regression

$$y = h_{\boldsymbol{\theta}}(\boldsymbol{x}) = \sigma(\boldsymbol{\theta}^T \boldsymbol{x})$$

where $\sigma(a) = \dfrac{1}{1 + \exp(-a)}$

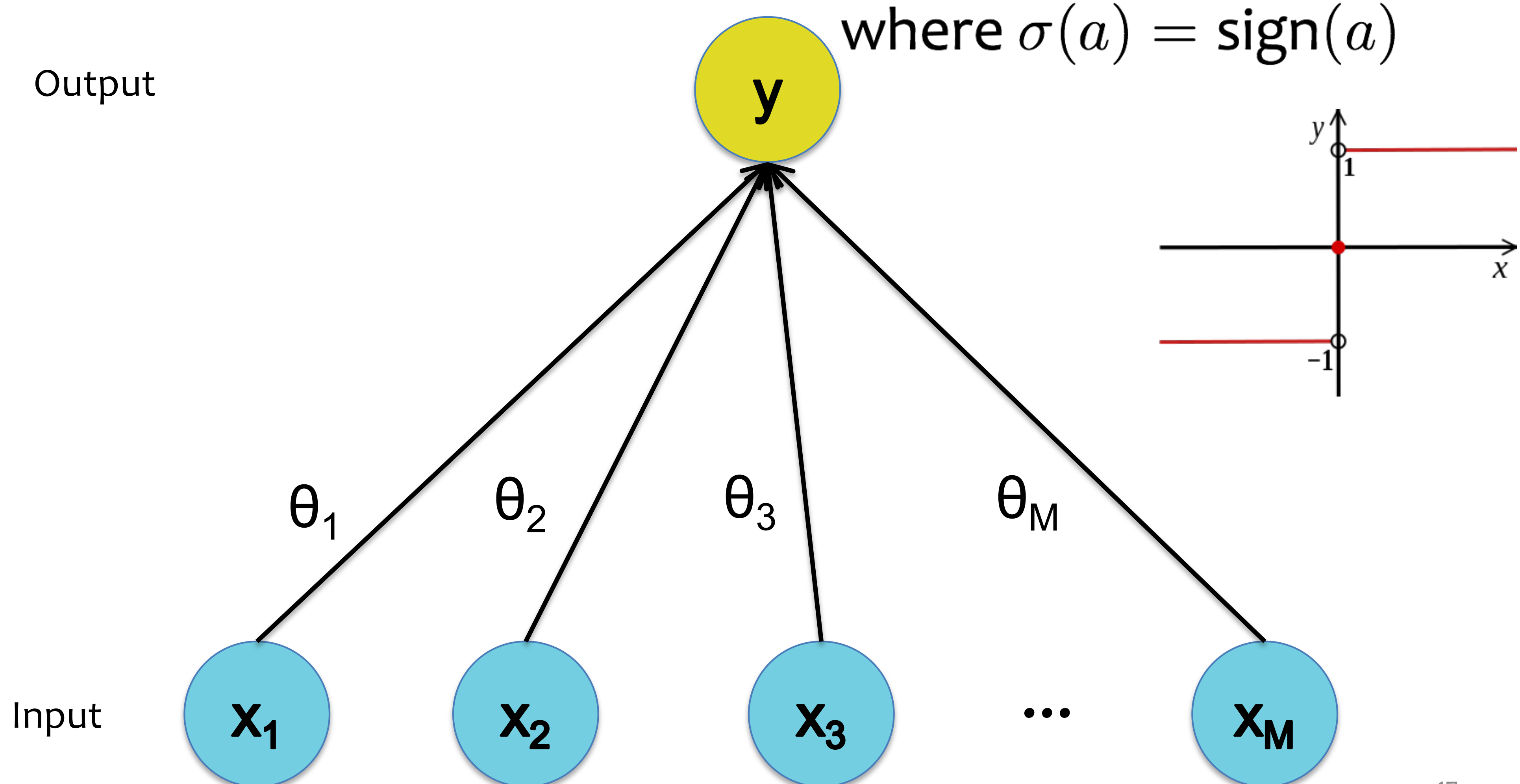


Decision Functions

Perceptron

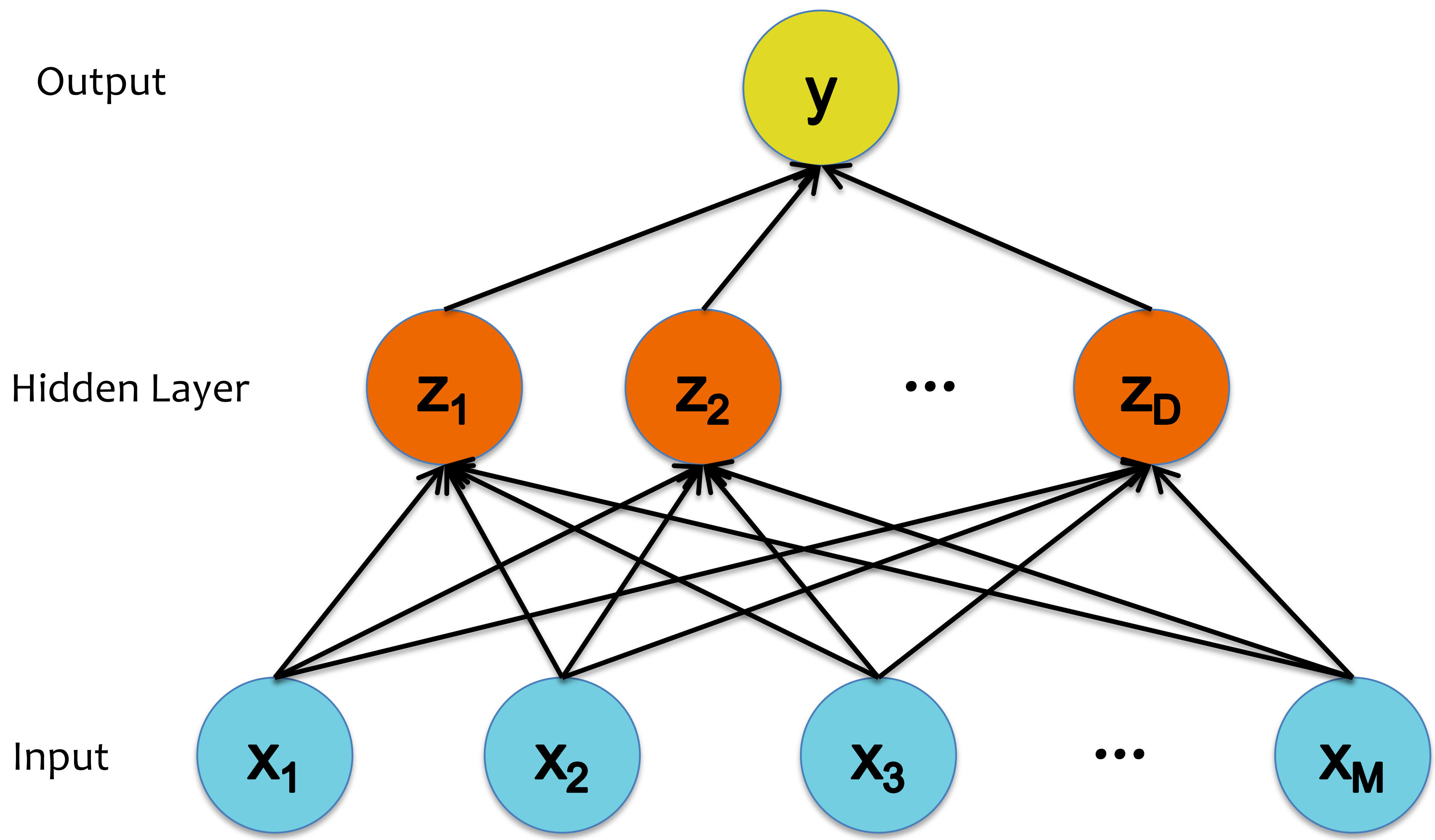
$$y = h_{\boldsymbol{\theta}}(\boldsymbol{x}) = \sigma(\boldsymbol{\theta}^T \boldsymbol{x})$$

where $\sigma(a) = \text{sign}(a)$



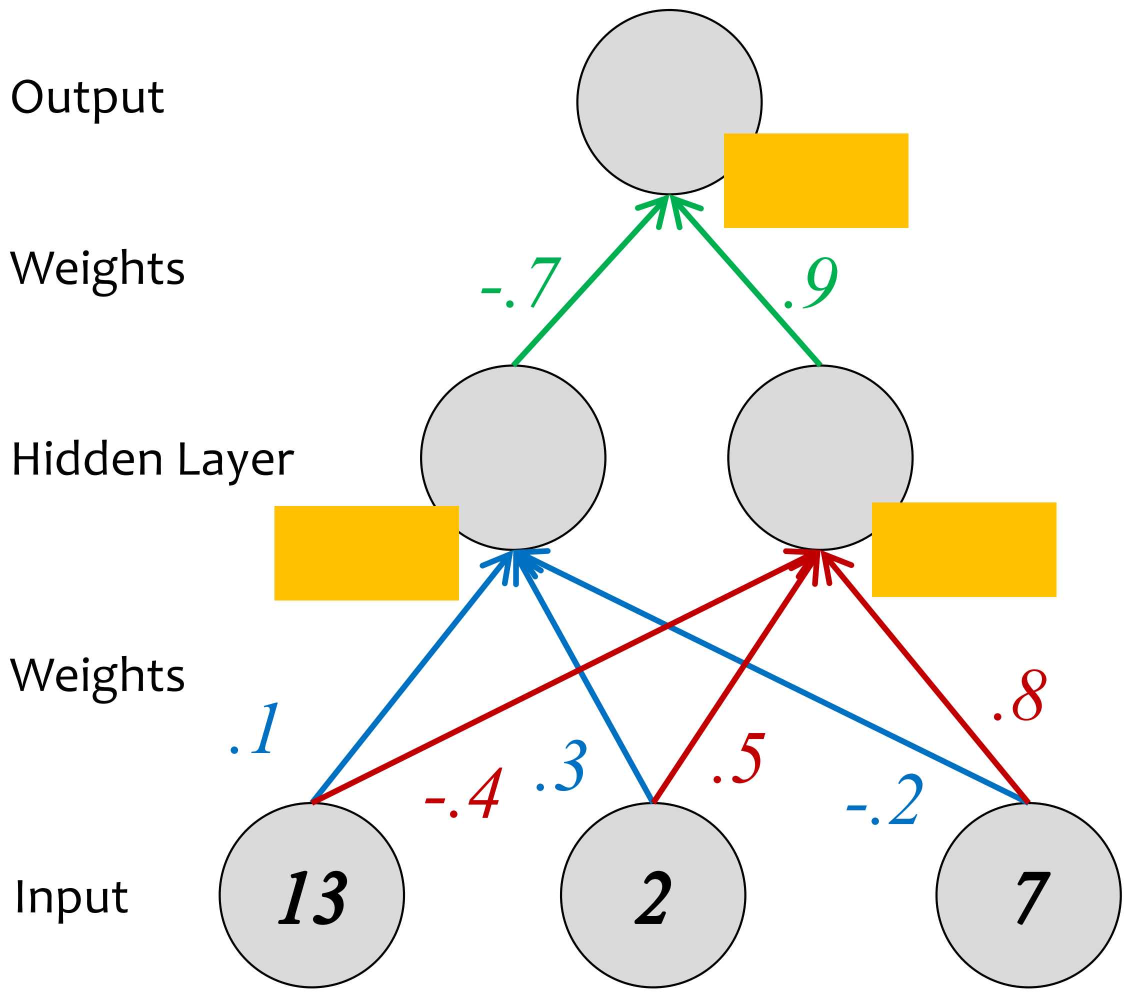
Decision Functions

Neural Network



COMPONENTS OF A NEURAL NETWORK

Neural Network

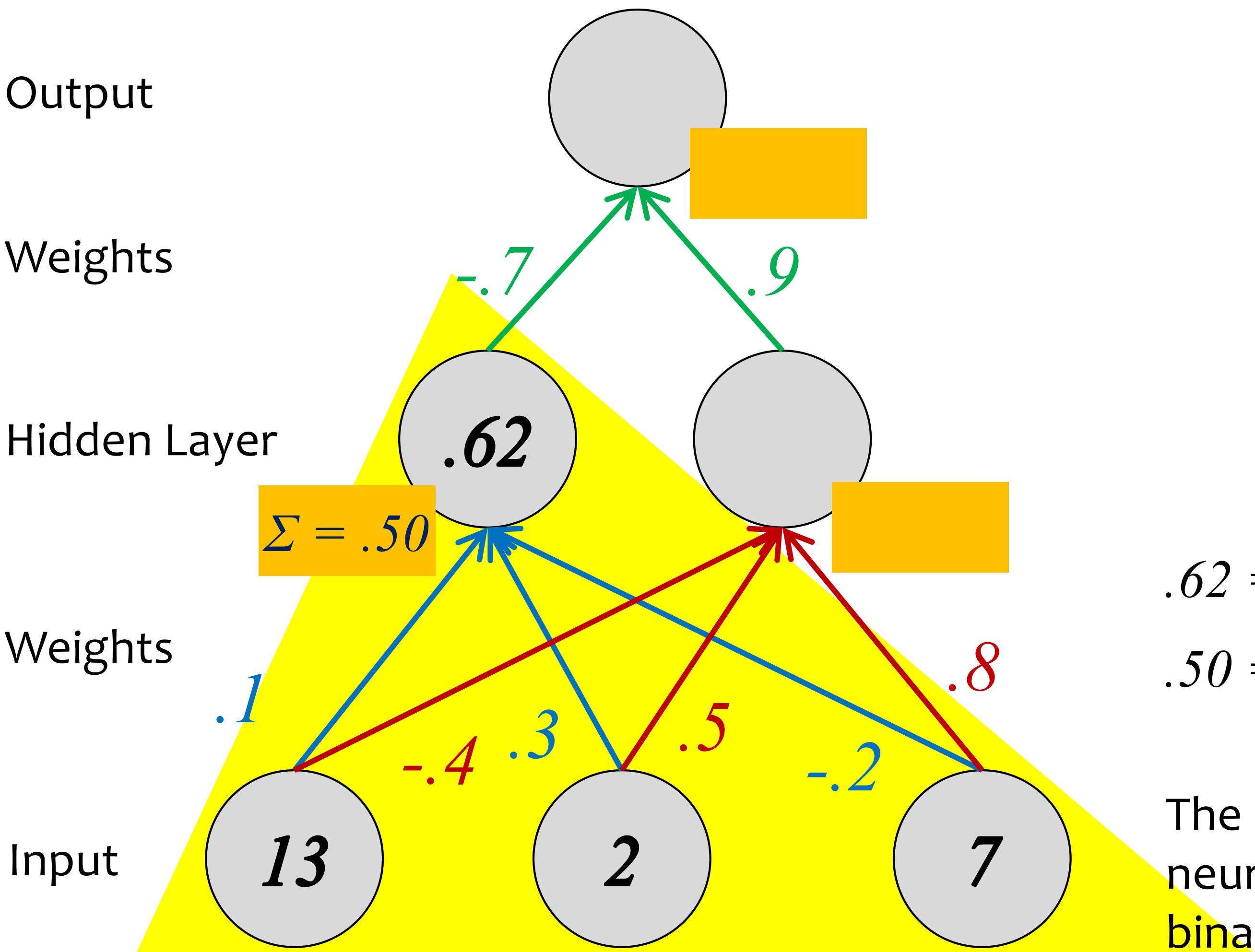


Suppose we already learned the weights of the neural network.

To make a new prediction, we take in some new features (aka. the input layer) and perform the feed-forward computation.

Decision Functions

Neural Network



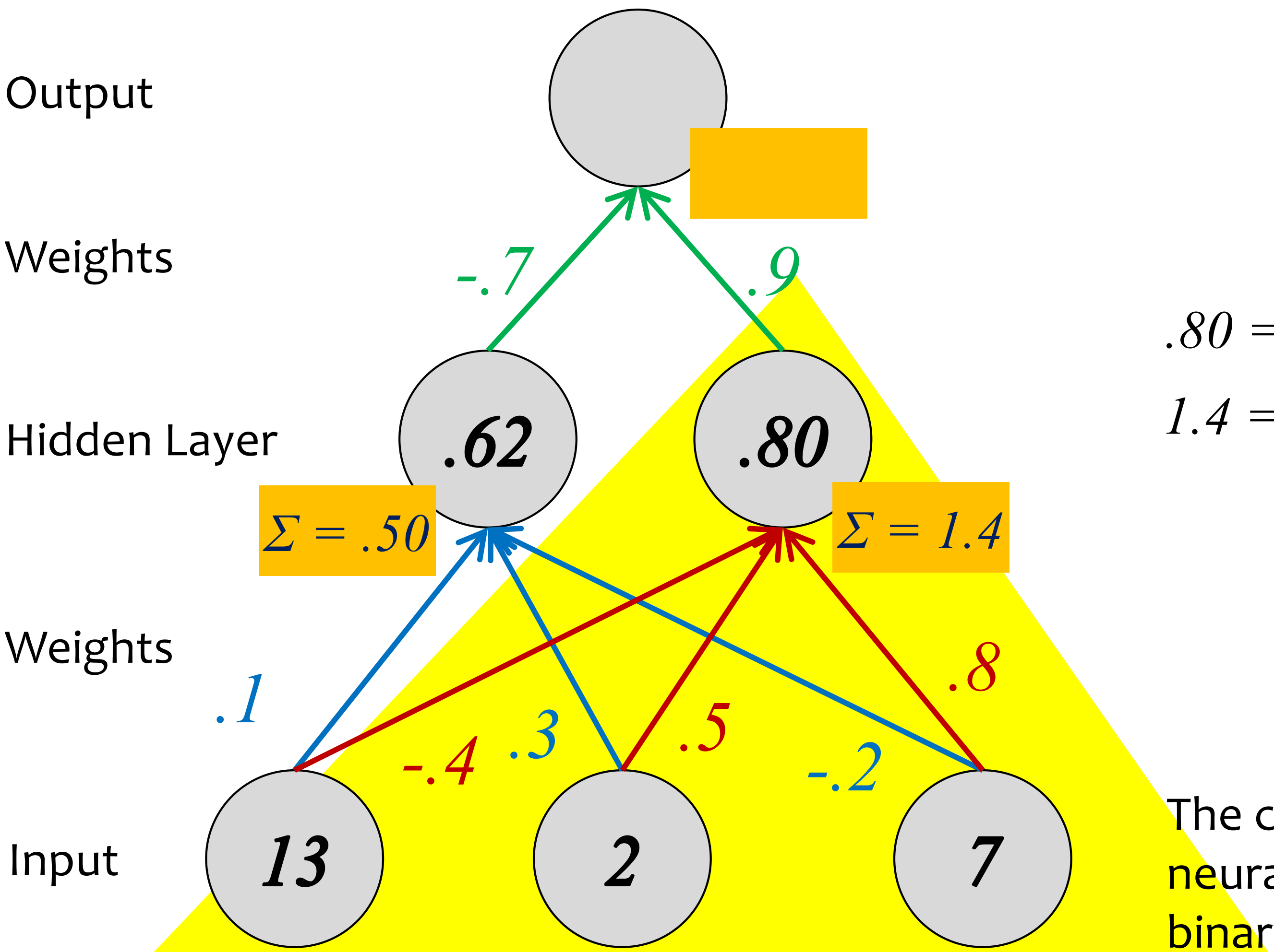
$.62 = \sigma(.50)$

$.50 = 13(.1) + 2(.3) + 7(-.2)$

The computation of each neural network unit resembles binary logistic regression.

Decision Functions

Neural Network



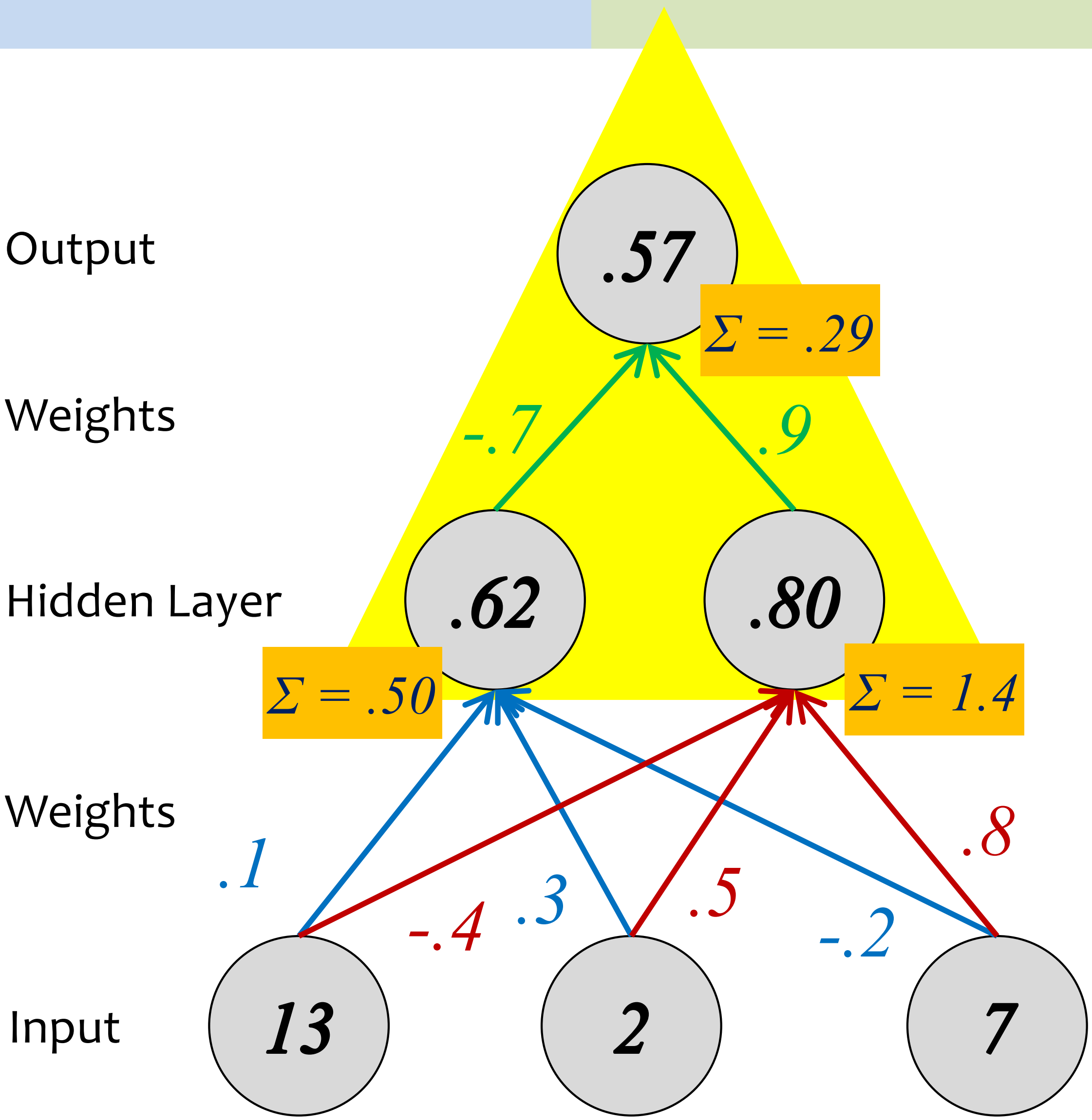
$.80 = \sigma(1.4)$

$1.4 = 13(-.4) + 2(.5) + 7(.8)$

The computation of each neural network unit resembles binary logistic regression.

Decision Functions

Neural Network



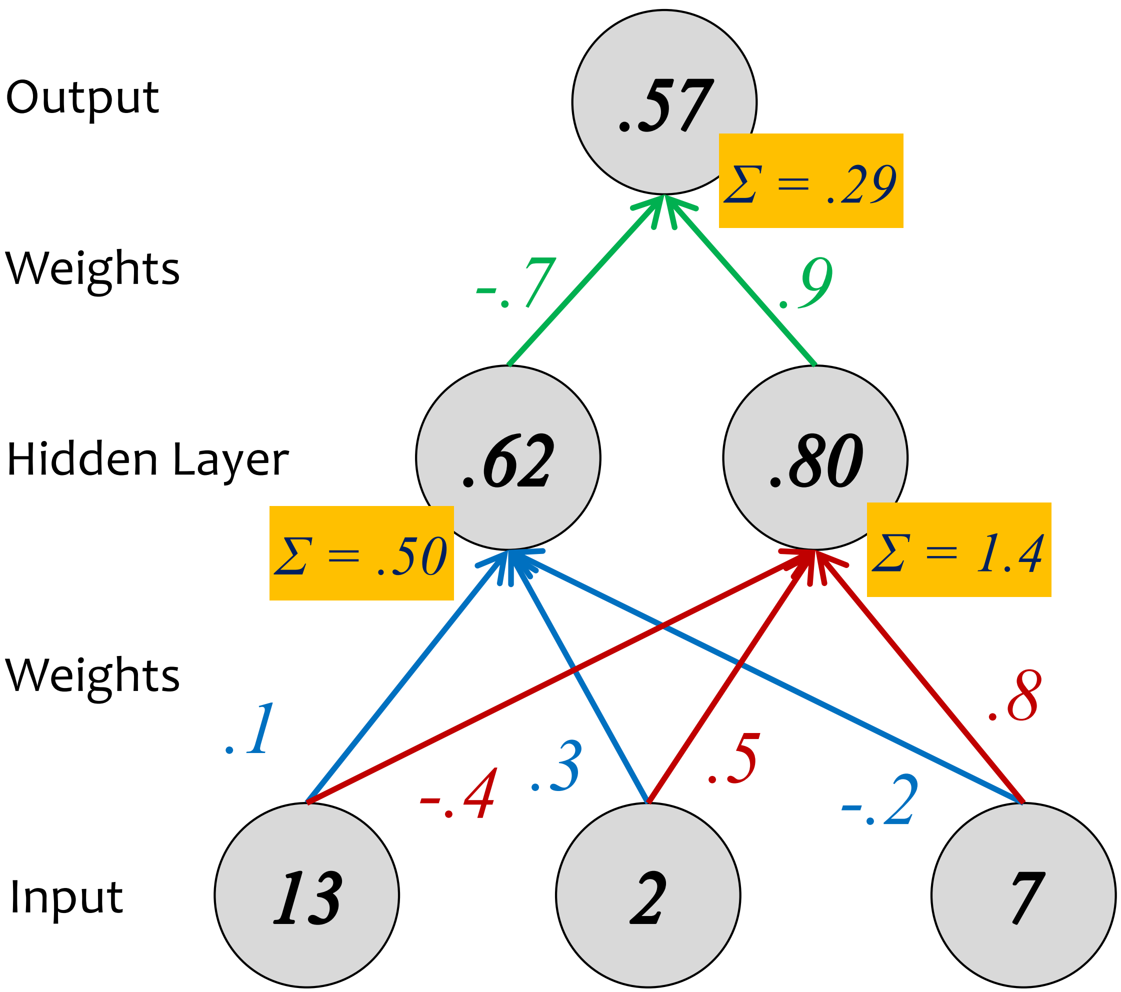
$.57 = \sigma(.29)$

$.29 = .62(-.7) + .80(.9)$

The computation of each neural network unit resembles binary logistic regression.

Decision Functions

Neural Network



$.57 = \sigma(.29)$

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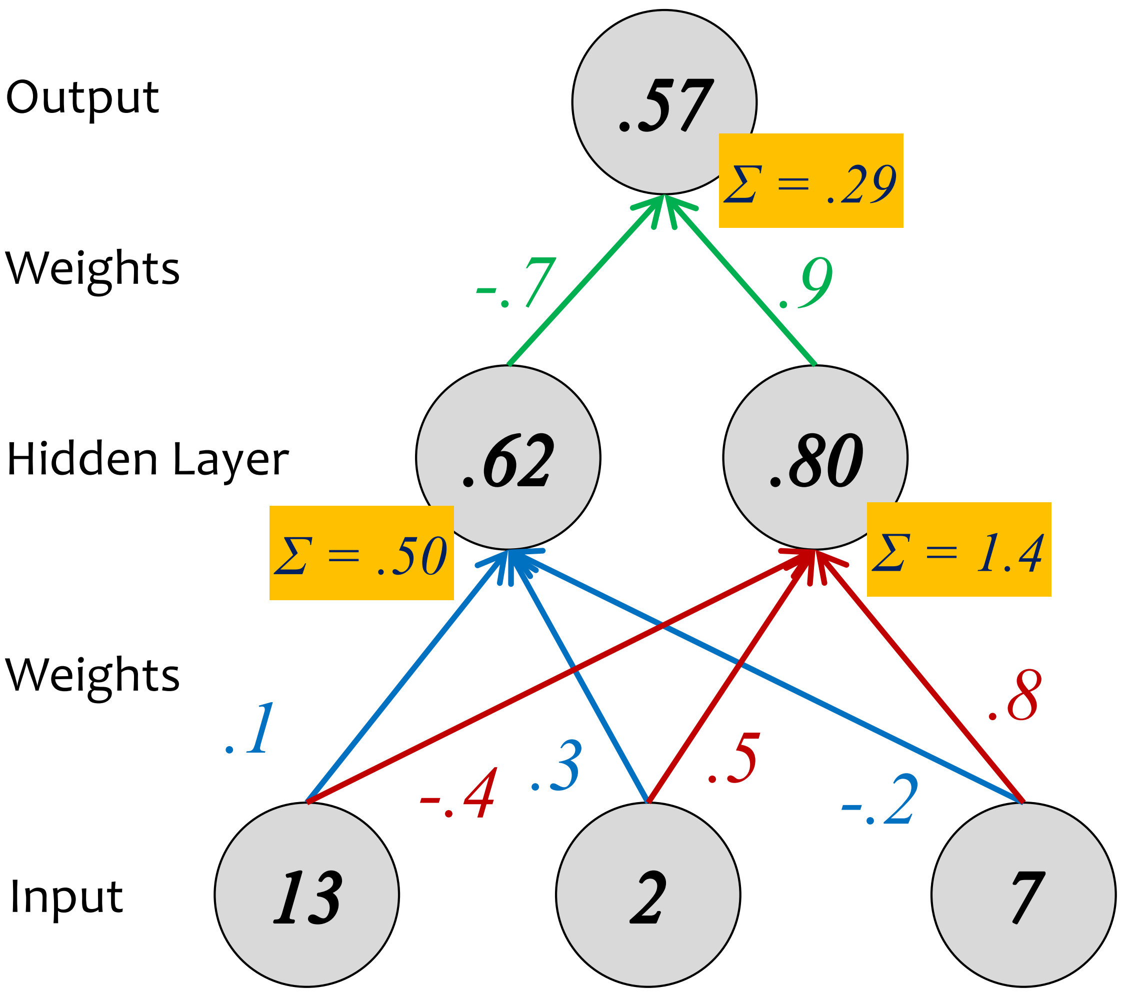
The computation of each neural network unit resembles binary logistic regression.

Decision Functions

Neural Network



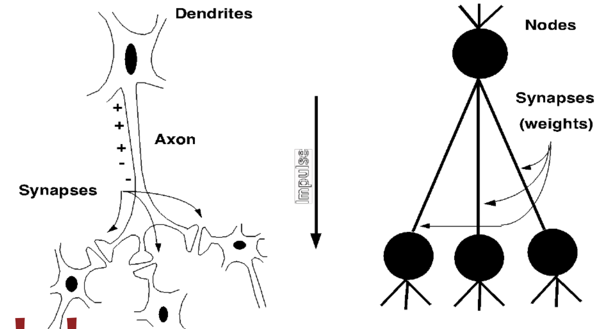
Except we only have the target value for y at training time!

We have to learn to create "useful" values of z_1 and z_2 in the hidden layer.

The computation of each neural network unit resembles binary logistic regression.

From Biological to Artificial

The motivation for Artificial Neural Networks comes from biology…



Biological "Model"

- **Neuron:** an excitable cell
- **Synapse:** connection between neurons
- A *neuron* sends an **electrochemical pulse** along its *synapses* when a sufficient voltage change occurs
- **Biological Neural Network:** collection of neurons along some pathway through the brain

Artificial Model

- **Neuron:** node in a directed acyclic graph (DAG)
- **Weight:** multiplier on each edge
- **Activation Function:** nonlinear thresholding function, which allows a neuron to "fire" when the input value is sufficiently high
- **Artificial Neural Network:** collection of neurons into a DAG, which define some differentiable function

Biological "Computation"

- Neuron switching time : ~ 0.001 sec
- Number of neurons: ~ 10^{10}
- Connections per neuron: ~ $10^{4\text{-}5}$
- Scene recognition time: ~ 0.1 sec

Artificial Computation

- Many neuron-like threshold switching units
- Many weighted interconnections among units
- Highly parallel, distributed processes

Slide adapted from Eric Xing

DEFINING A 1-HIDDEN LAYER NEURAL NETWORK

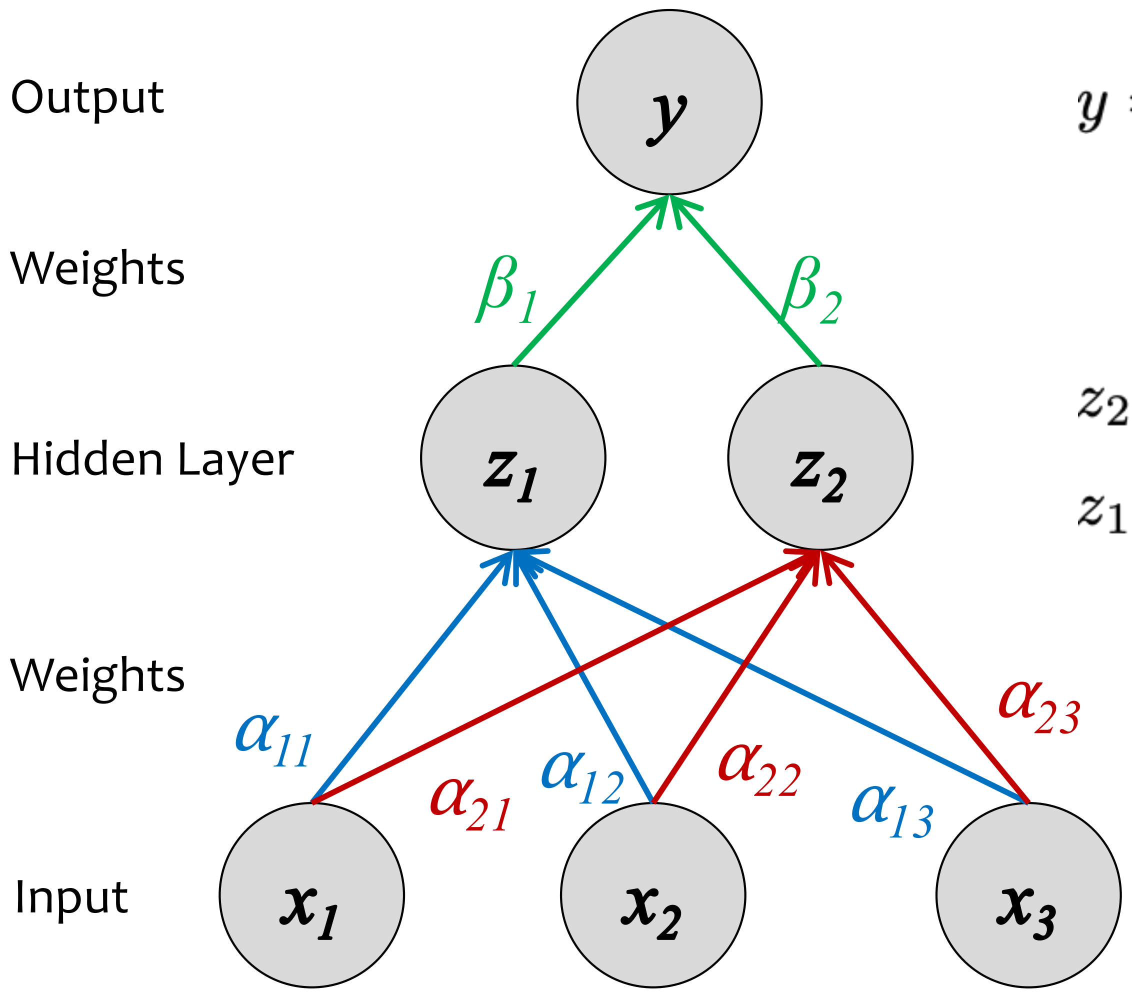
Neural Networks

Chalkboard

- Example: Neural Network w/1 Hidden Layer

Decision Functions

Neural Network



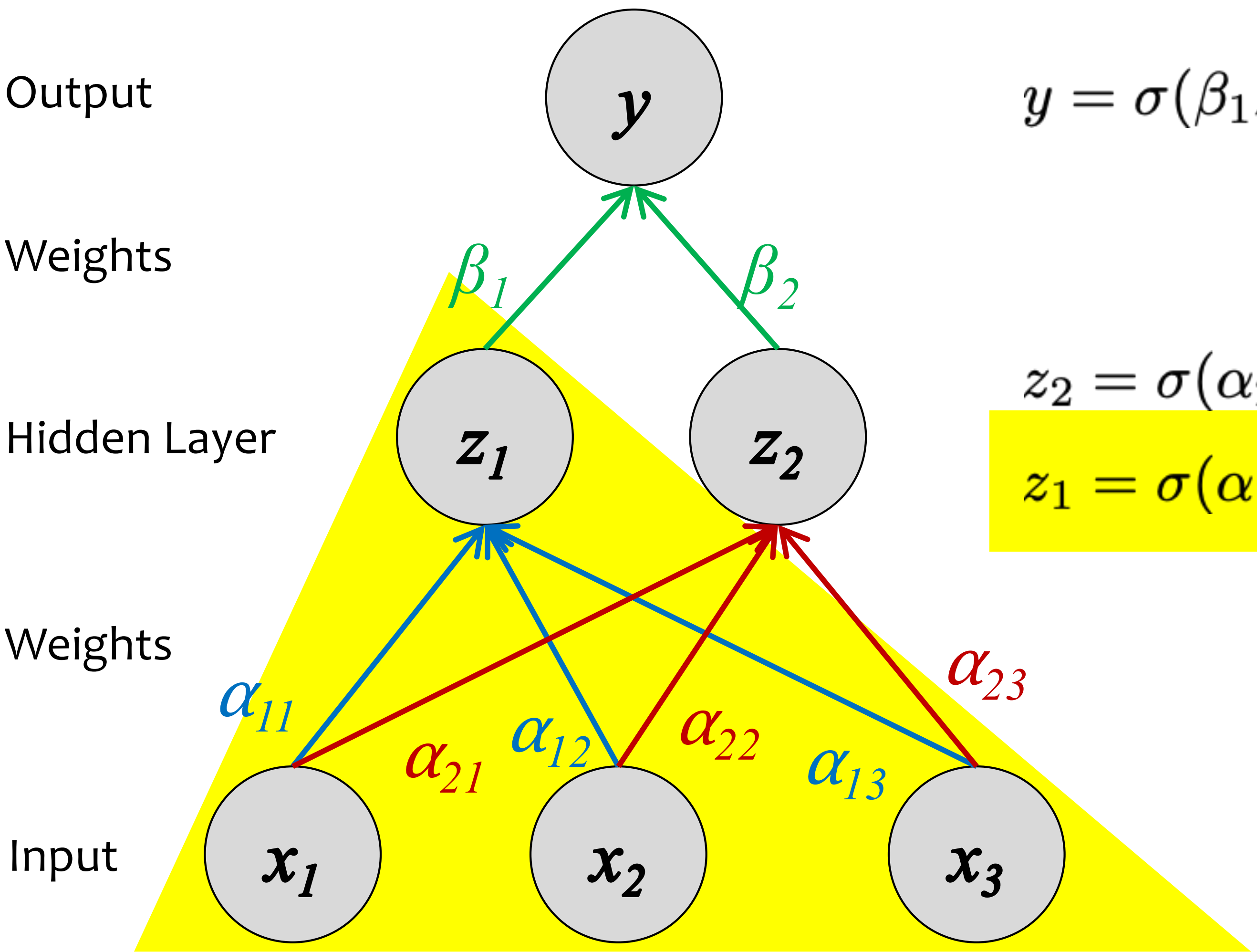
$$y = \sigma(\beta_1 z_1 + \beta_2 z_2)$$

$$z_2 = \sigma(\alpha_{21} x_1 + \alpha_{22} x_2 + \alpha_{23} x_3)$$

$$z_1 = \sigma(\alpha_{11} x_1 + \alpha_{12} x_2 + \alpha_{13} x_3)$$

Decision Functions

Neural Network



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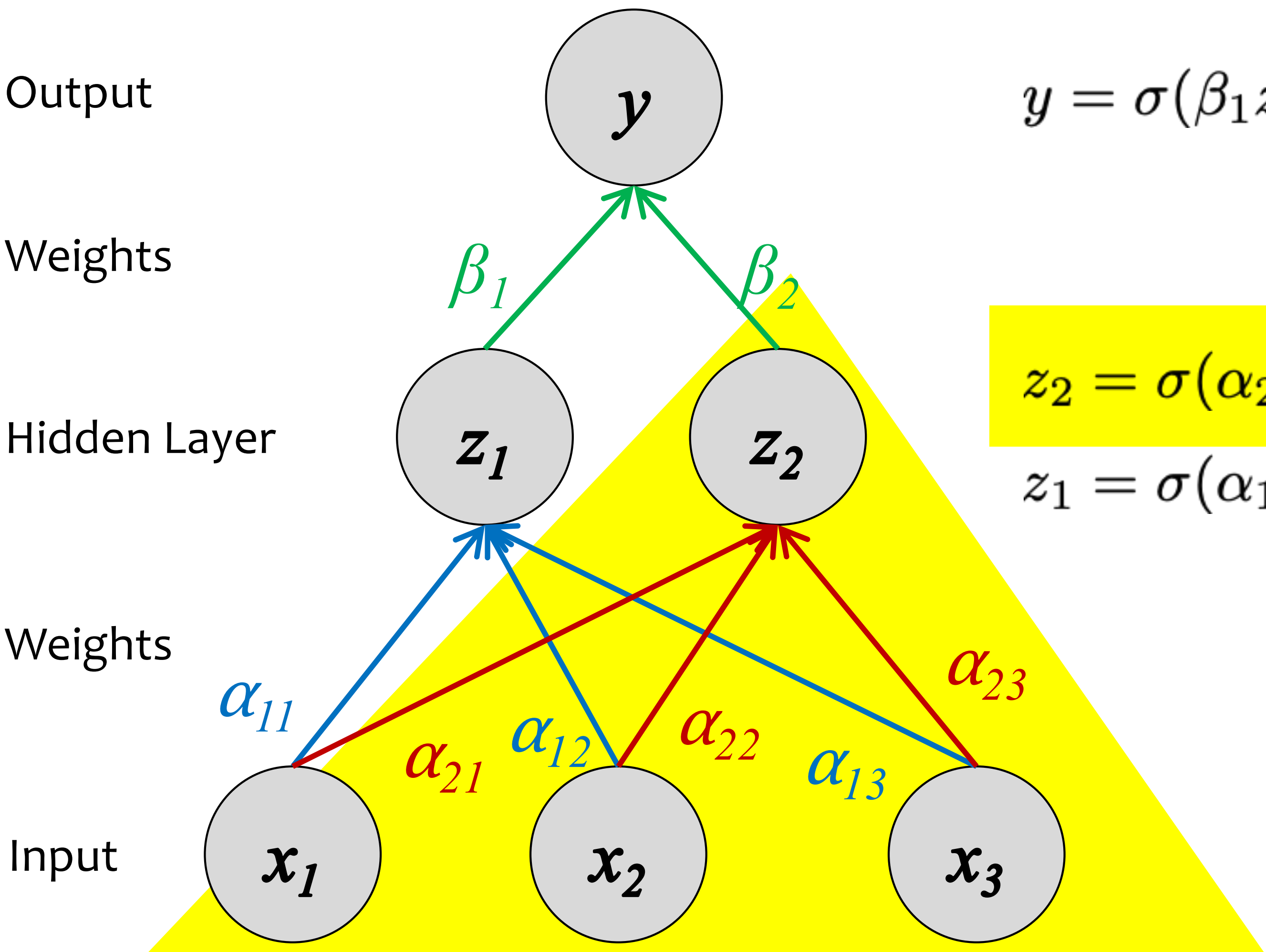
Decision Functions

Neural Network



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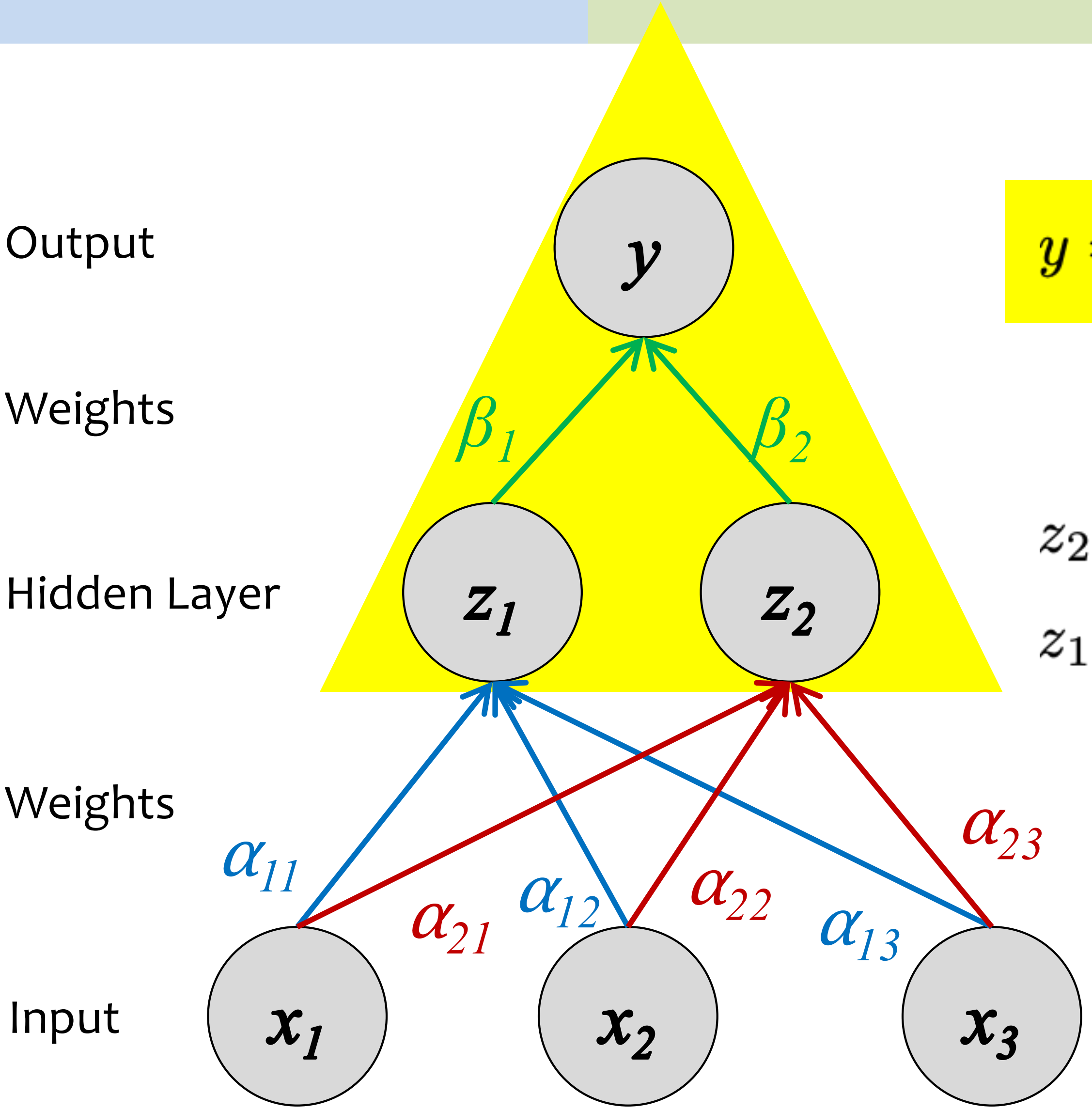
Neural Network



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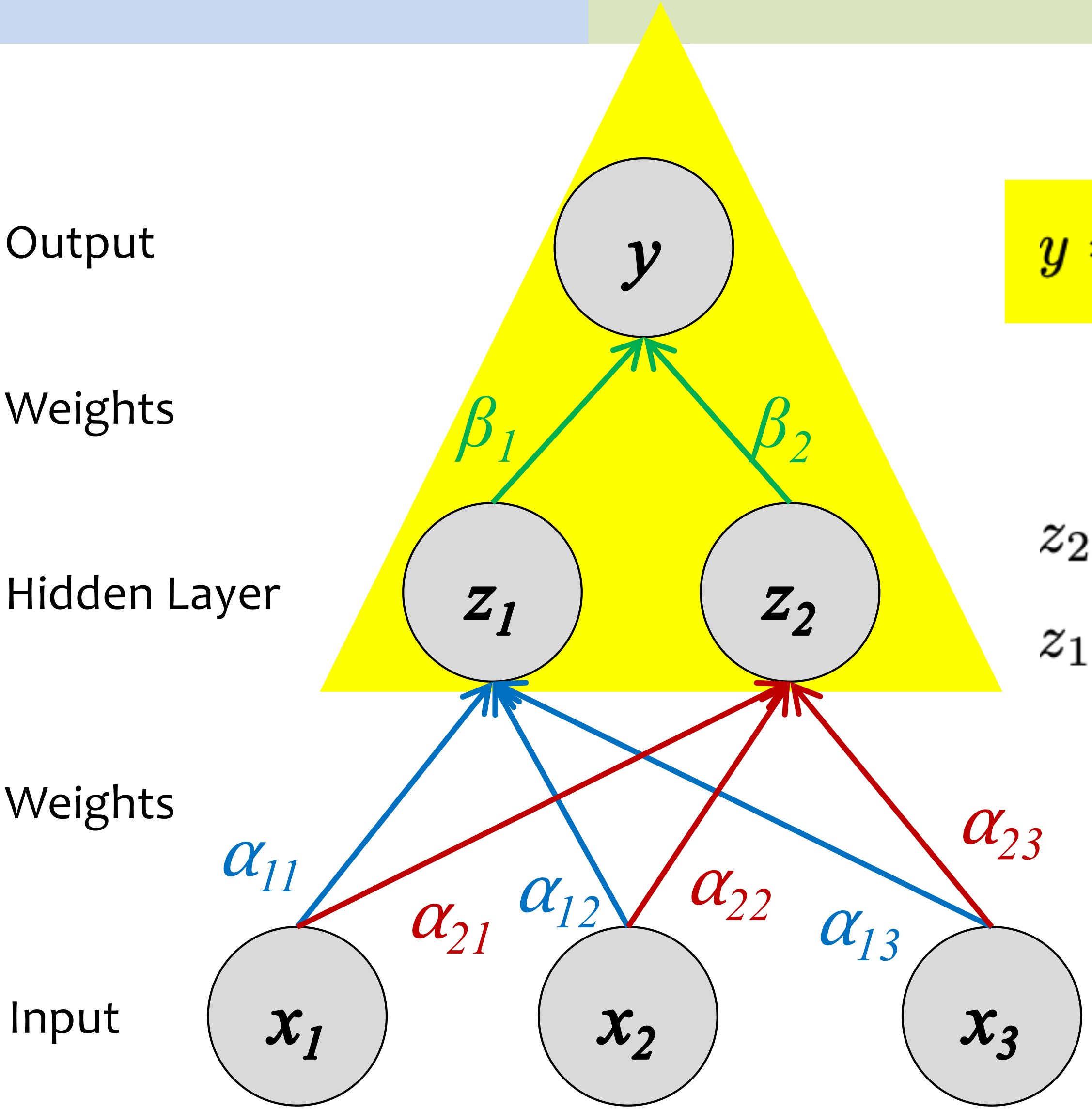
Decision Functions

Neural Network



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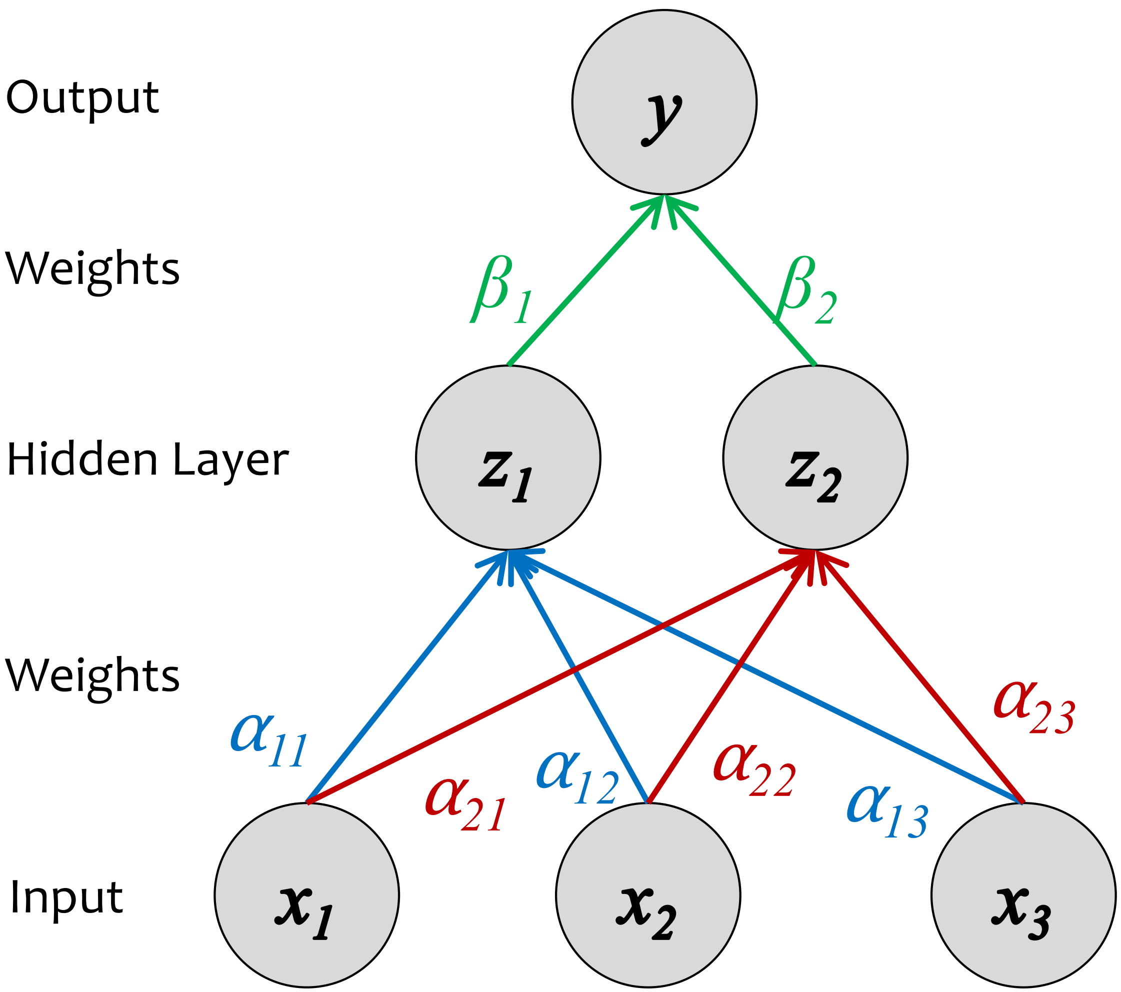
Decision Functions

Neural Network



$$y = \sigma(\boldsymbol{\beta}^T \mathbf{z})$$

$$z_2 = \sigma(\boldsymbol{\alpha}_{2,\cdot}^T \mathbf{x})$$

$$z_1 = \sigma(\boldsymbol{\alpha}_{1,\cdot}^T \mathbf{x})$$

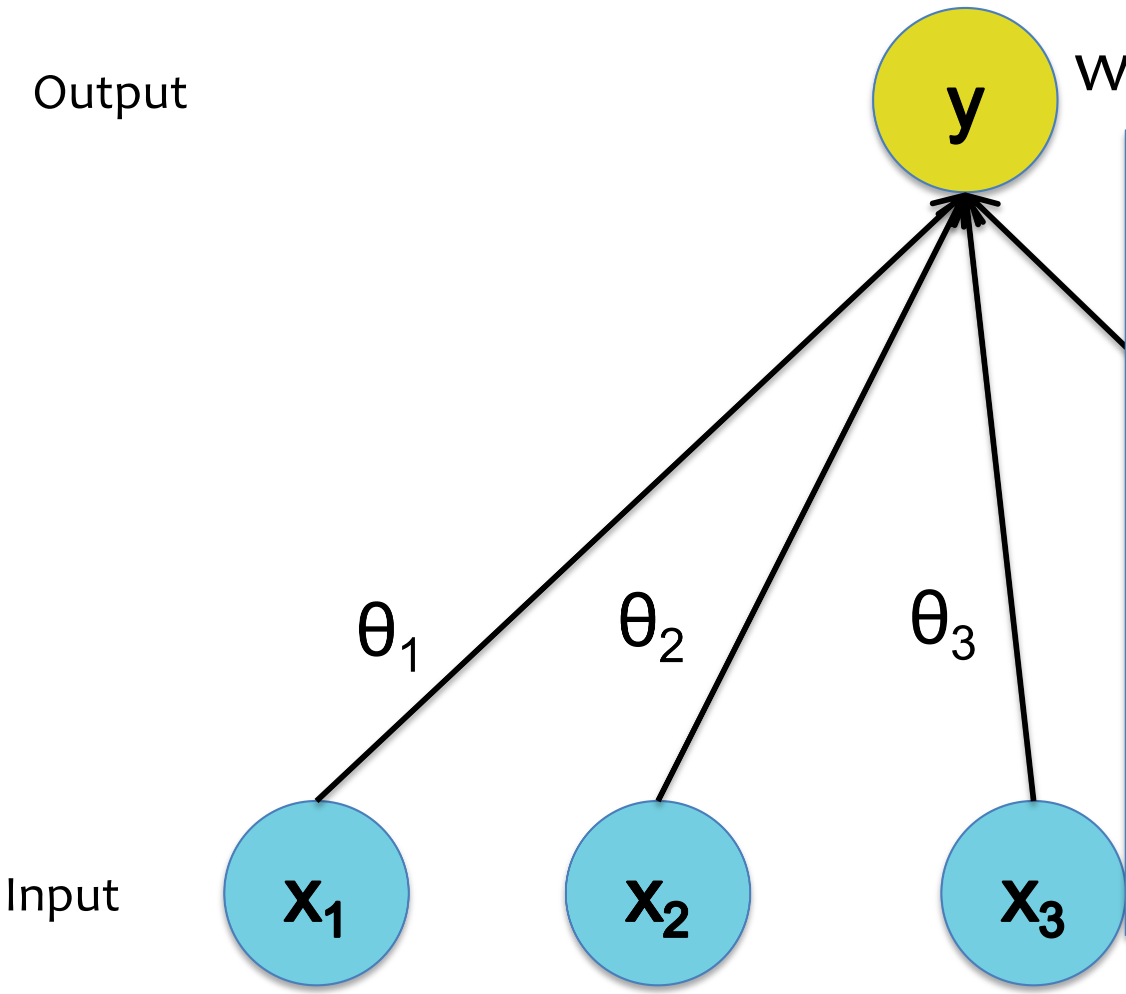
NONLINEAR DECISION BOUNDARIES AND NEURAL NETWORKS

Decision Functions

Logistic Regression

$$y = h_{\boldsymbol{\theta}}(\boldsymbol{x}) = \sigma(\boldsymbol{\theta}^T \boldsymbol{x})$$

where $\sigma(a) = \dfrac{1}{1+\exp(-a)}$



Decision Functions

Logistic Regression

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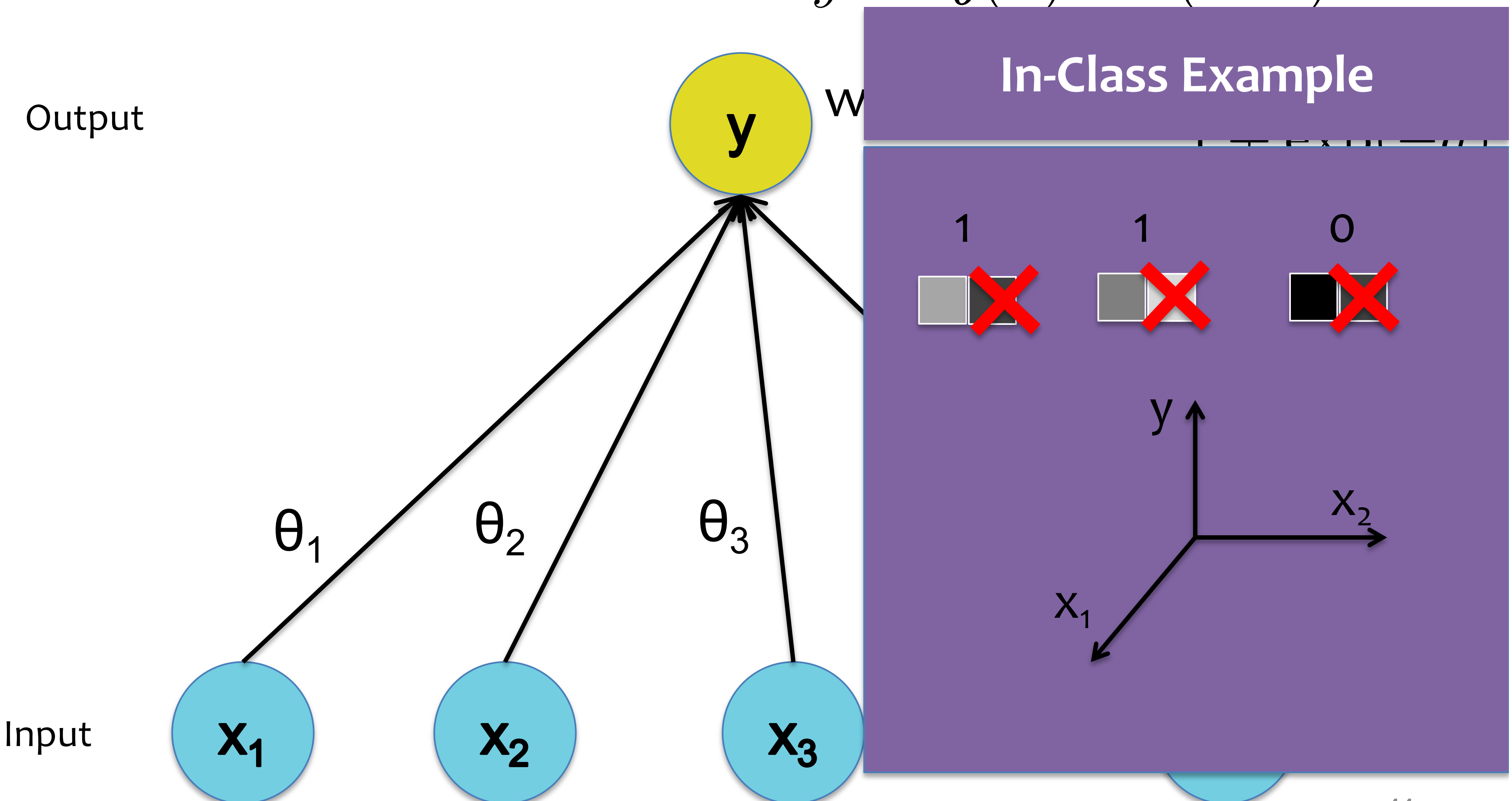


Neural Networks

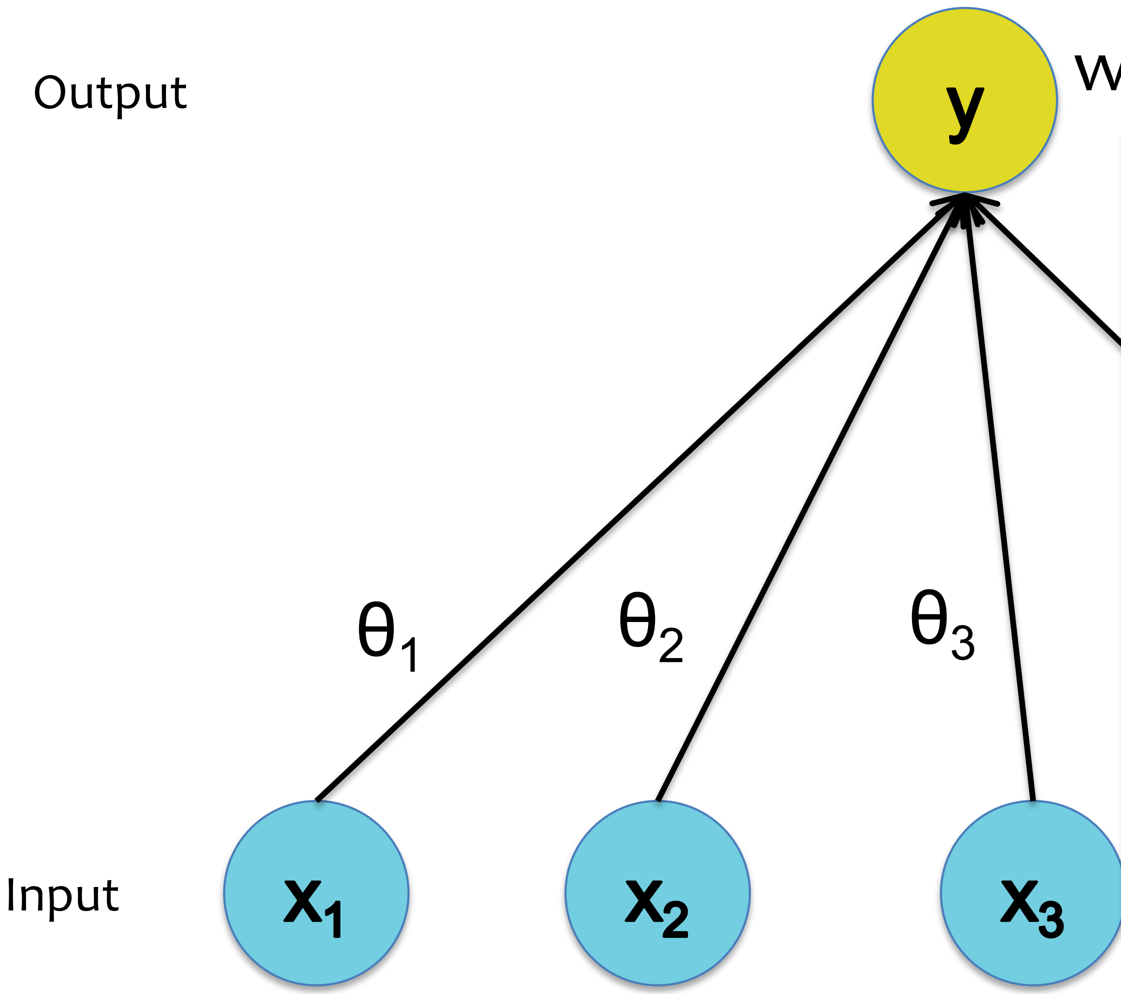
Chalkboard

- 1D Example from linear regression to logistic regression
- 1D Example from logistic regression to a neural network

Logistic Regression

$$y = h_{\boldsymbol{\theta}}(\boldsymbol{x}) = \sigma(\boldsymbol{\theta}^T \boldsymbol{x})$$

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



Decision Functions

Logistic Regression

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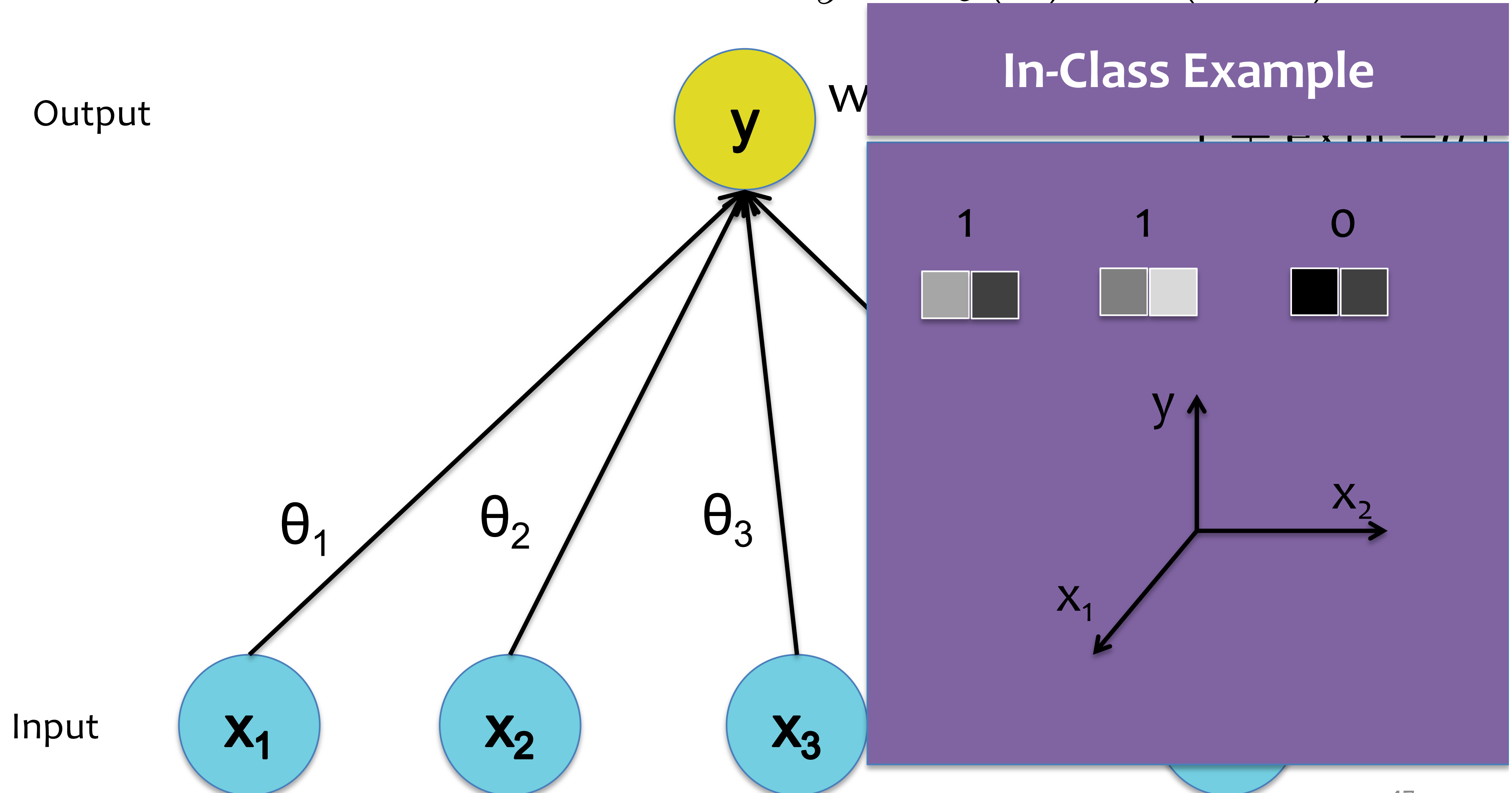
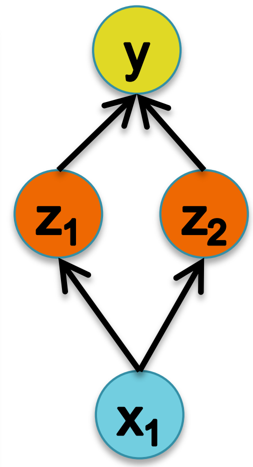


Neural Network Parameters

Question:

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

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

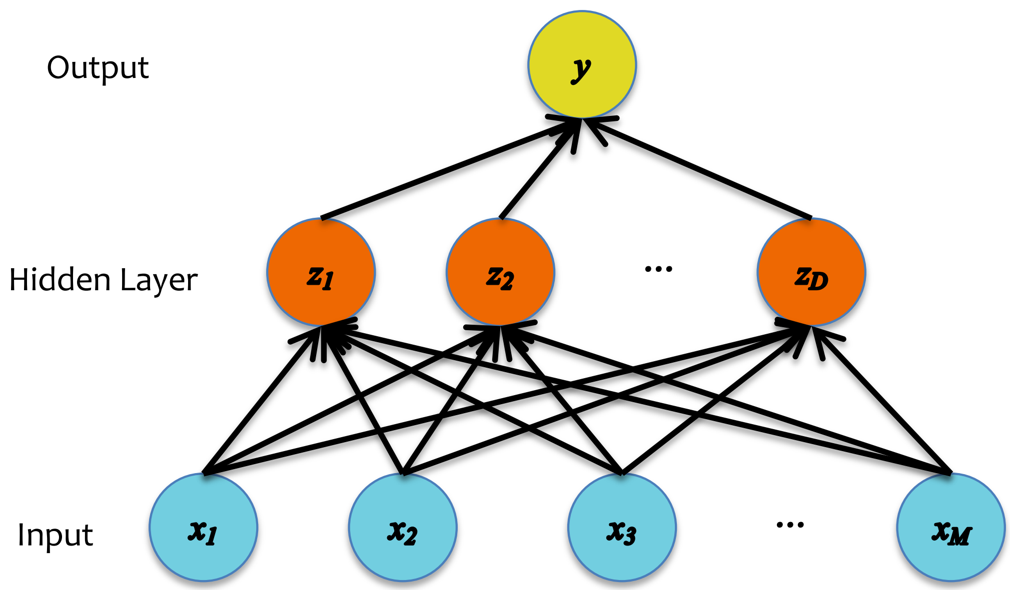


Answer:

ARCHITECTURES

Neural Network

Neural Network for Classification



(E) **Output (sigmoid)**
$y = \frac{1}{1+\exp(-b)}$

(D) **Output (linear)**
$b = \sum_{j=0}^{D} \beta_j z_j$

(C) **Hidden (sigmoid)**
$z_j = \frac{1}{1+\exp(-a_j)}, \ \forall j$

(B) **Hidden (linear)**
$a_j = \sum_{i=0}^{M} \alpha_{ji} x_i, \ \forall j$

(A) **Input**
Given $x_i, \ \forall i$

Neural Networks

Chalkboard

- Example: Neural Network w/2 Hidden Layers
- Example: Feed Forward Neural Network (matrix form)

Neural Network Architectures

Even for a basic Neural Network, there are many design decisions to make:

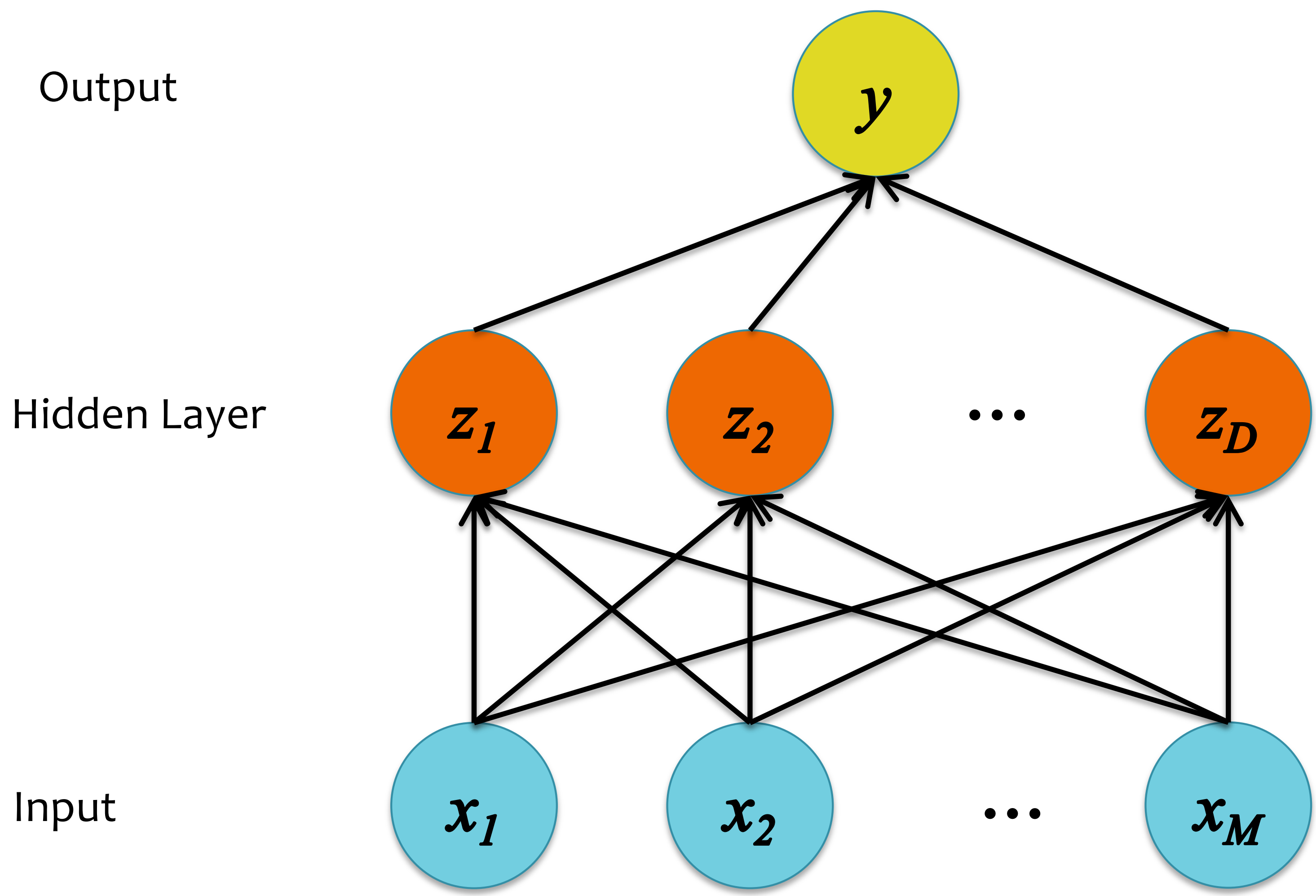
1. # of hidden layers (depth)
2. # of units per hidden layer (width)
3. Type of activation function (nonlinearity)
4. Form of objective function
5. How to initialize the parameters

BUILDING WIDER NETWORKS

D = M

Building a Neural Net

Q: How many hidden units, D, should we use?



The hidden units could learn to be…

- a selection of the most useful features
- nonlinear combinations of the features
- a lower dimensional projection of the features
- a higher dimensional projection of the features
- a copy of the input features
- a mix of the above

D < M

Building a Neural Net

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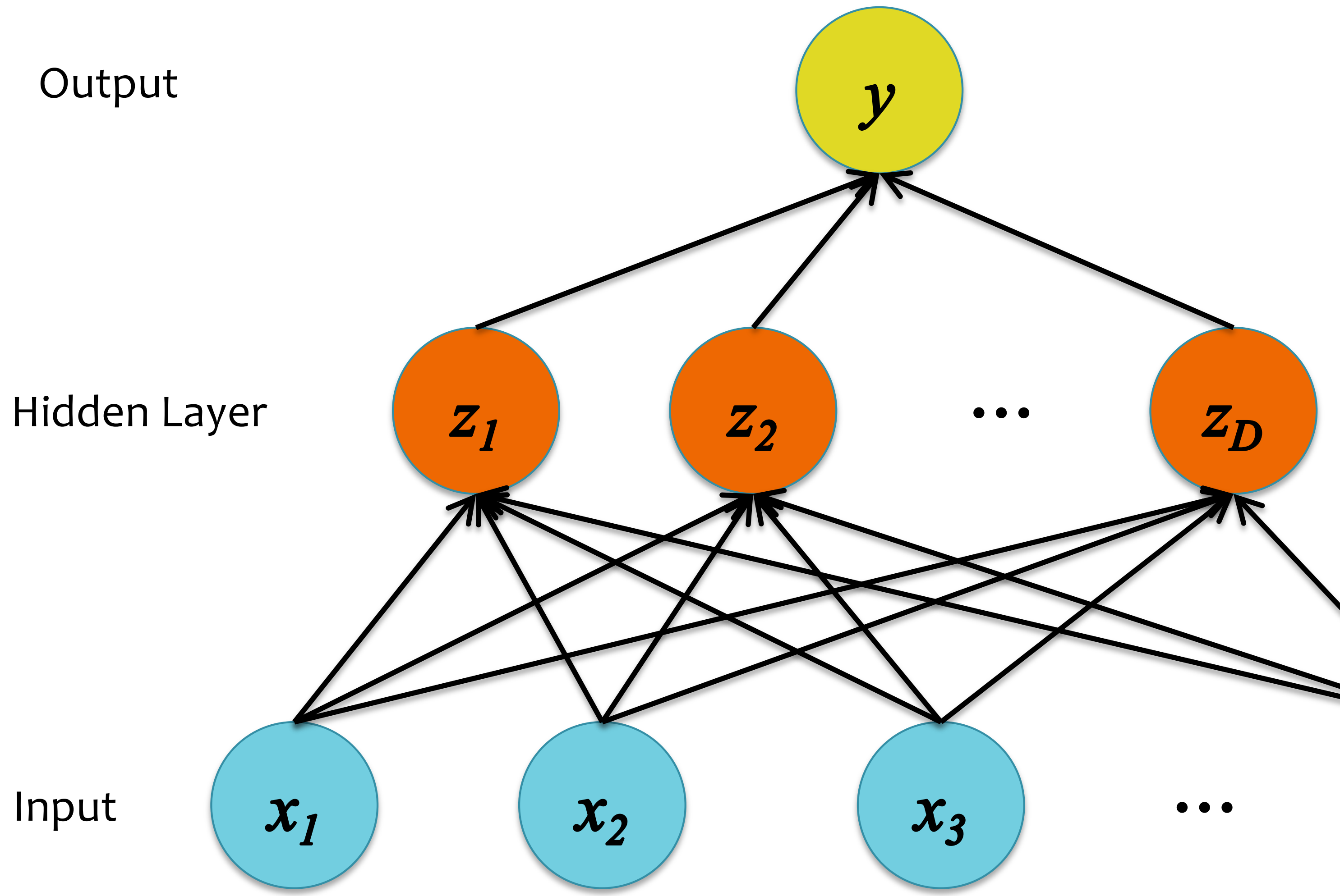

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D > M

Building a Neural Net

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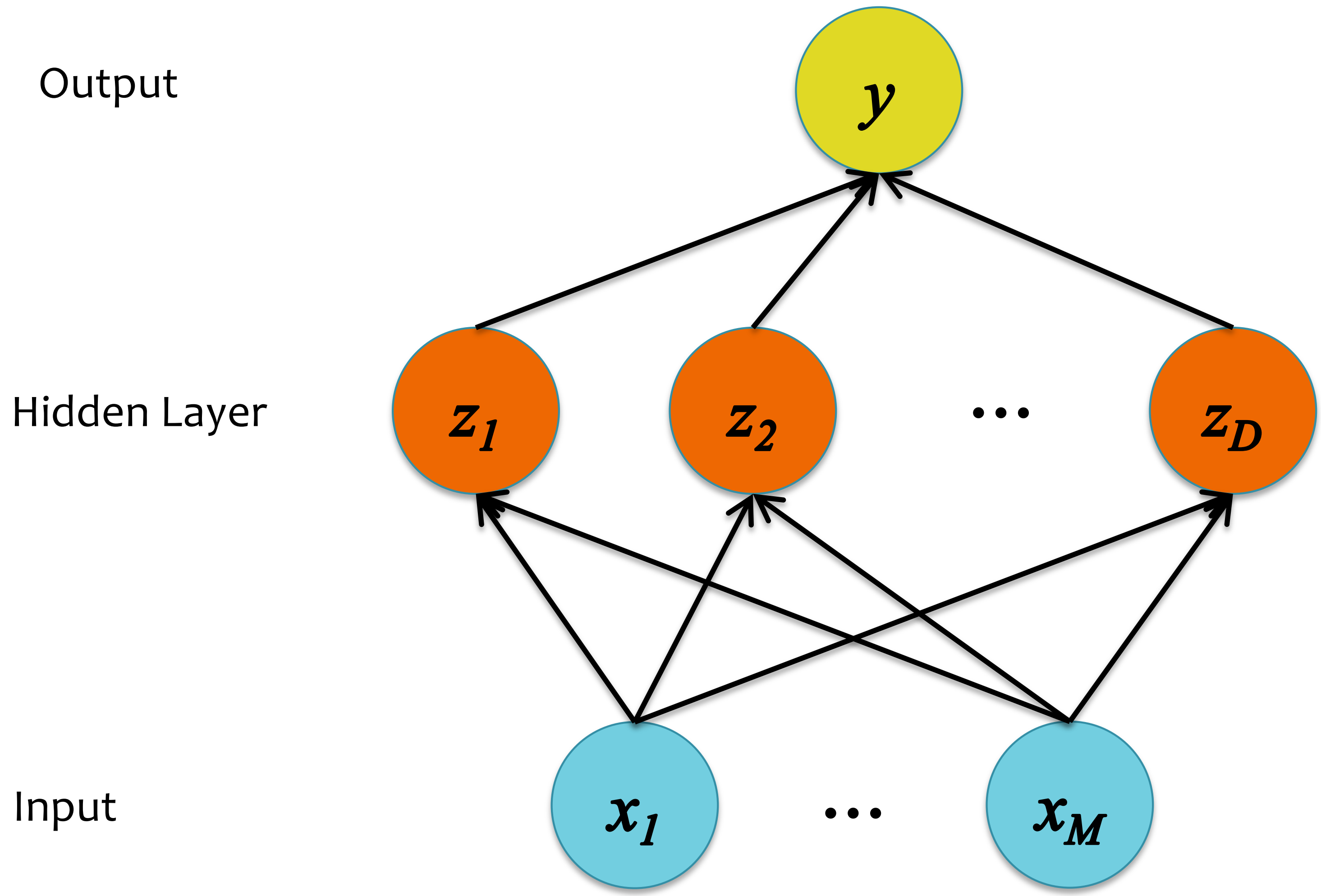

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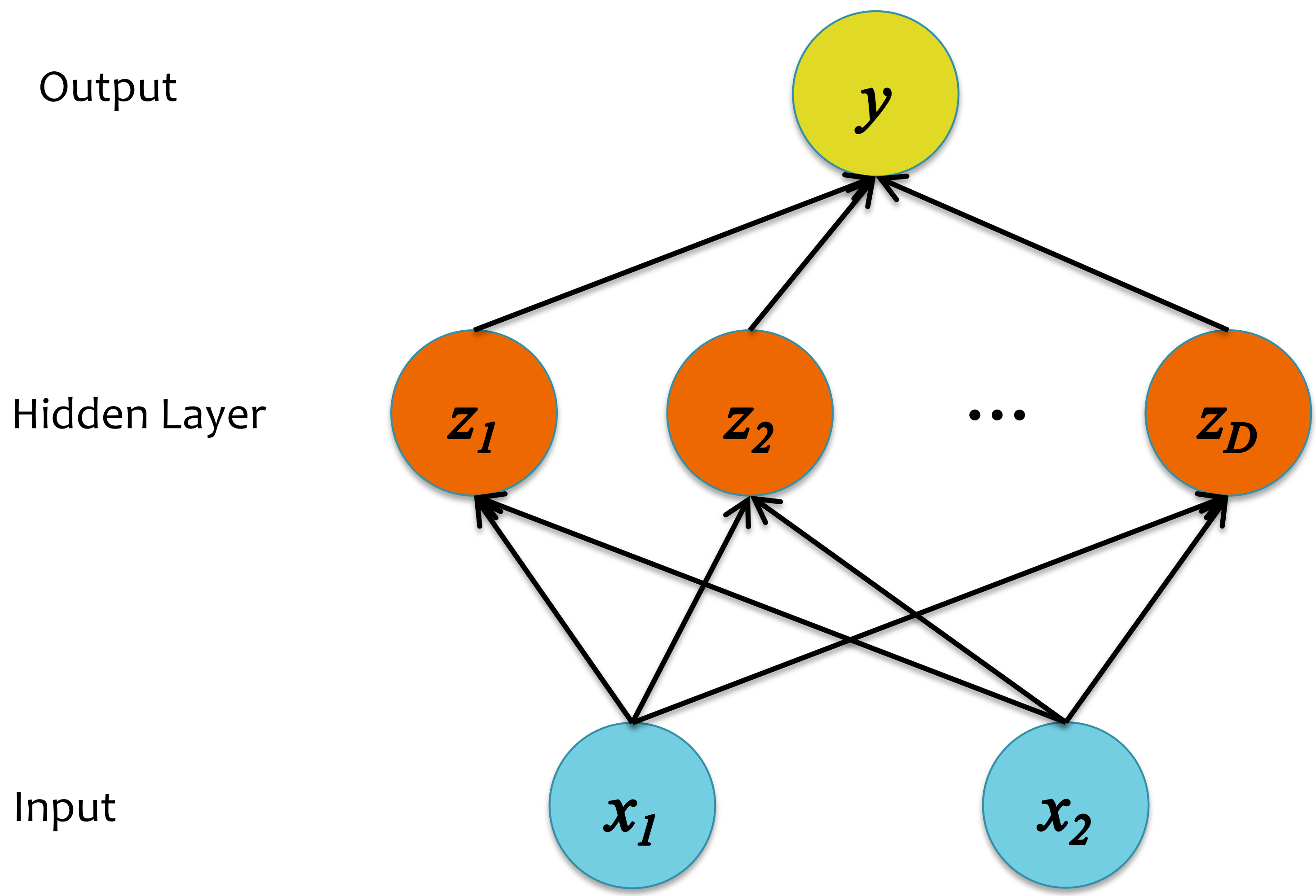
D ≥ M

Building a Neural Net

In the following examples, we have two input features, M=2, and we vary the number of hidden units, D.



The hidden units could learn to be…

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- nonlinear combinations of the features
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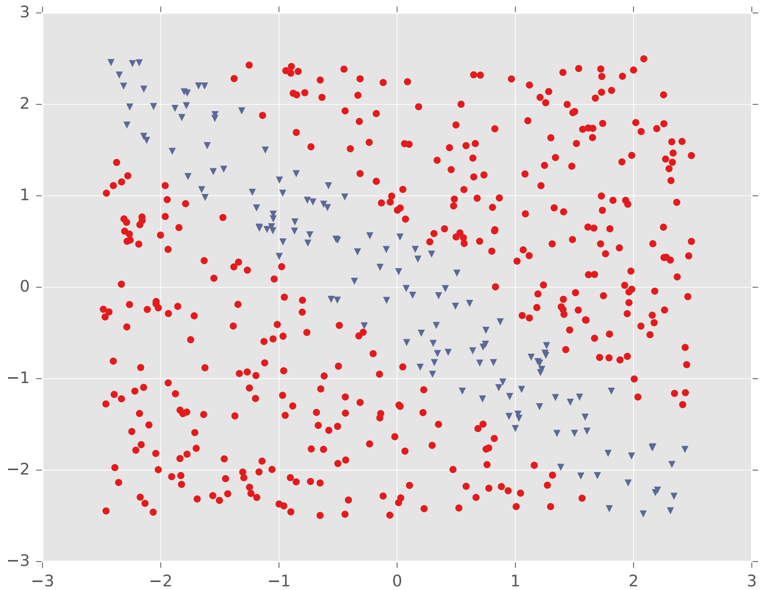
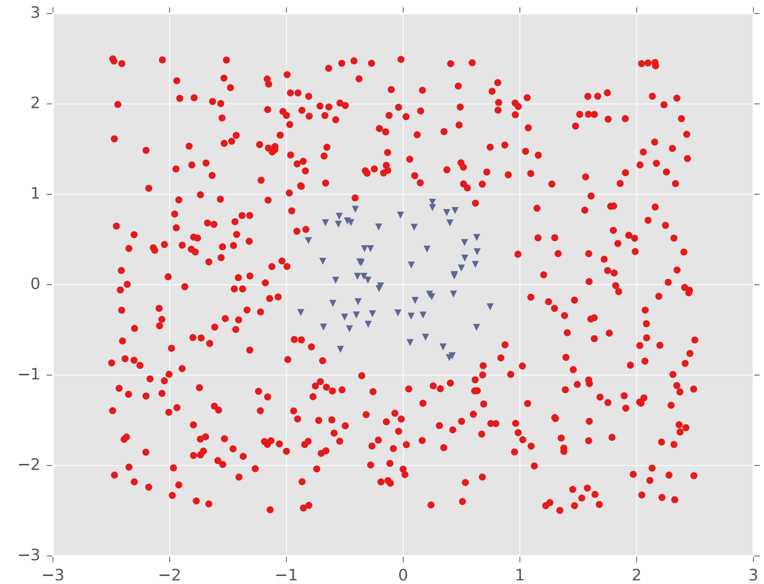
Examples 1 and 2

DECISION BOUNDARY EXAMPLES

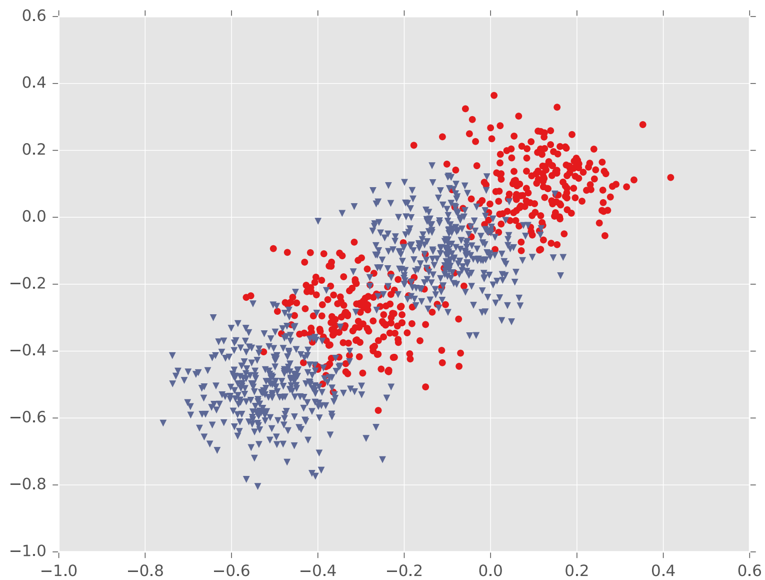
Example #1: Diagonal Band



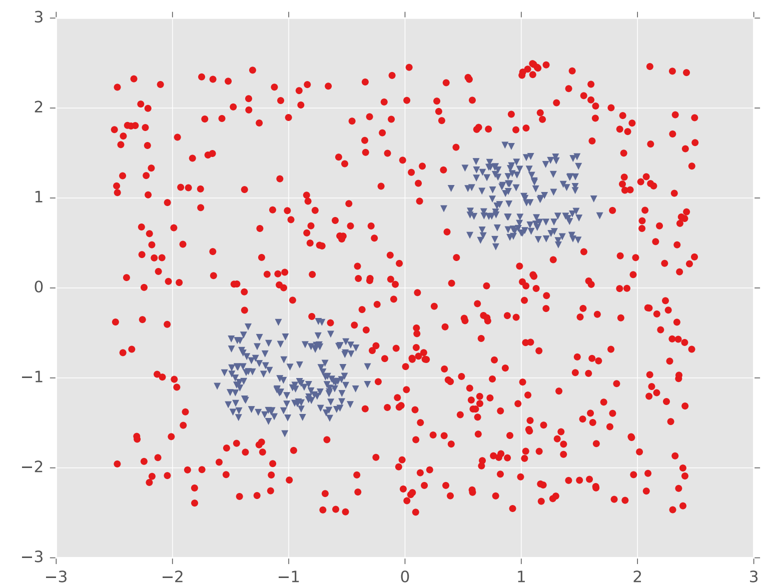
Example #2: One Pocket



Example #3: Four Gaussians



Example #4: Two Pockets



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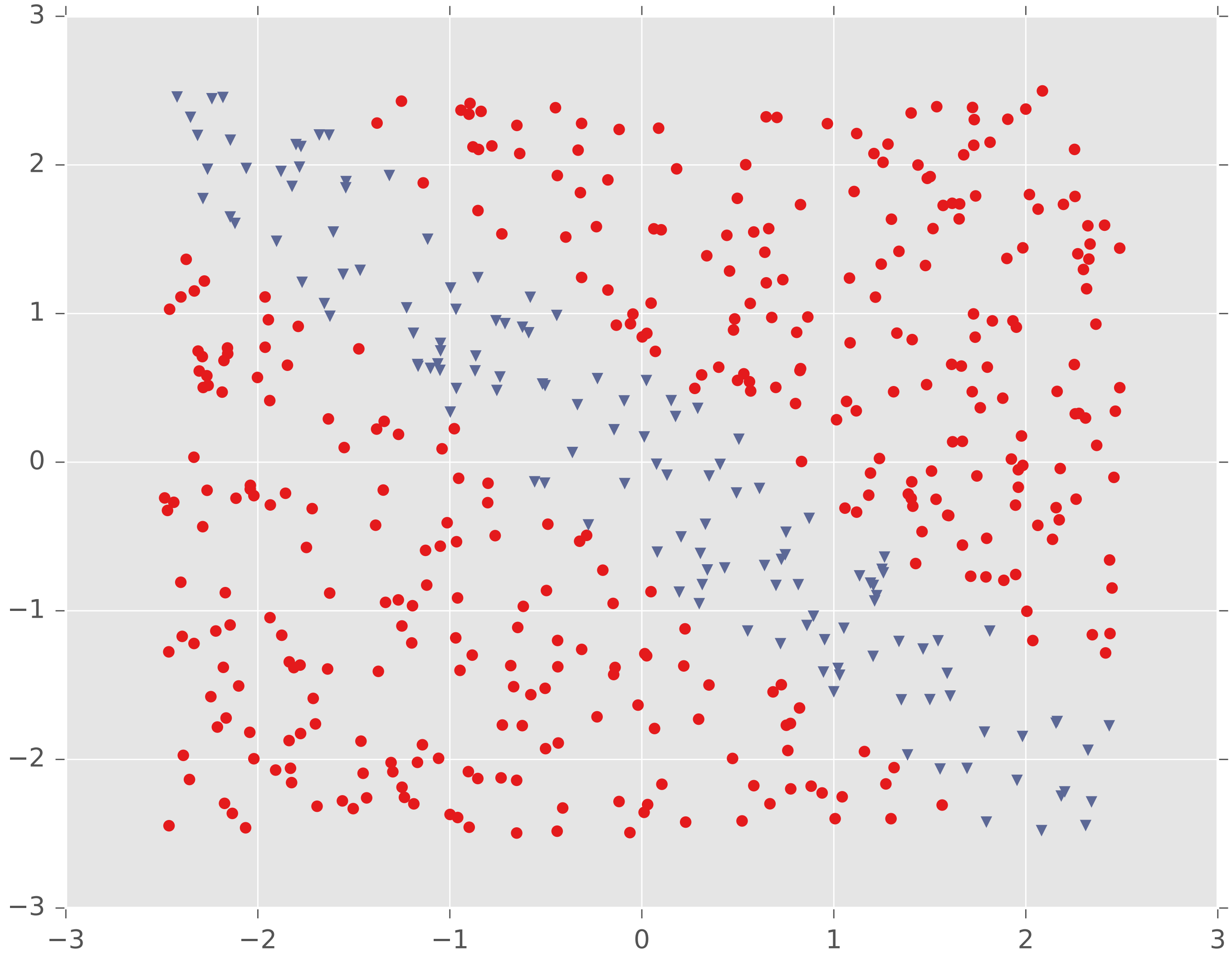

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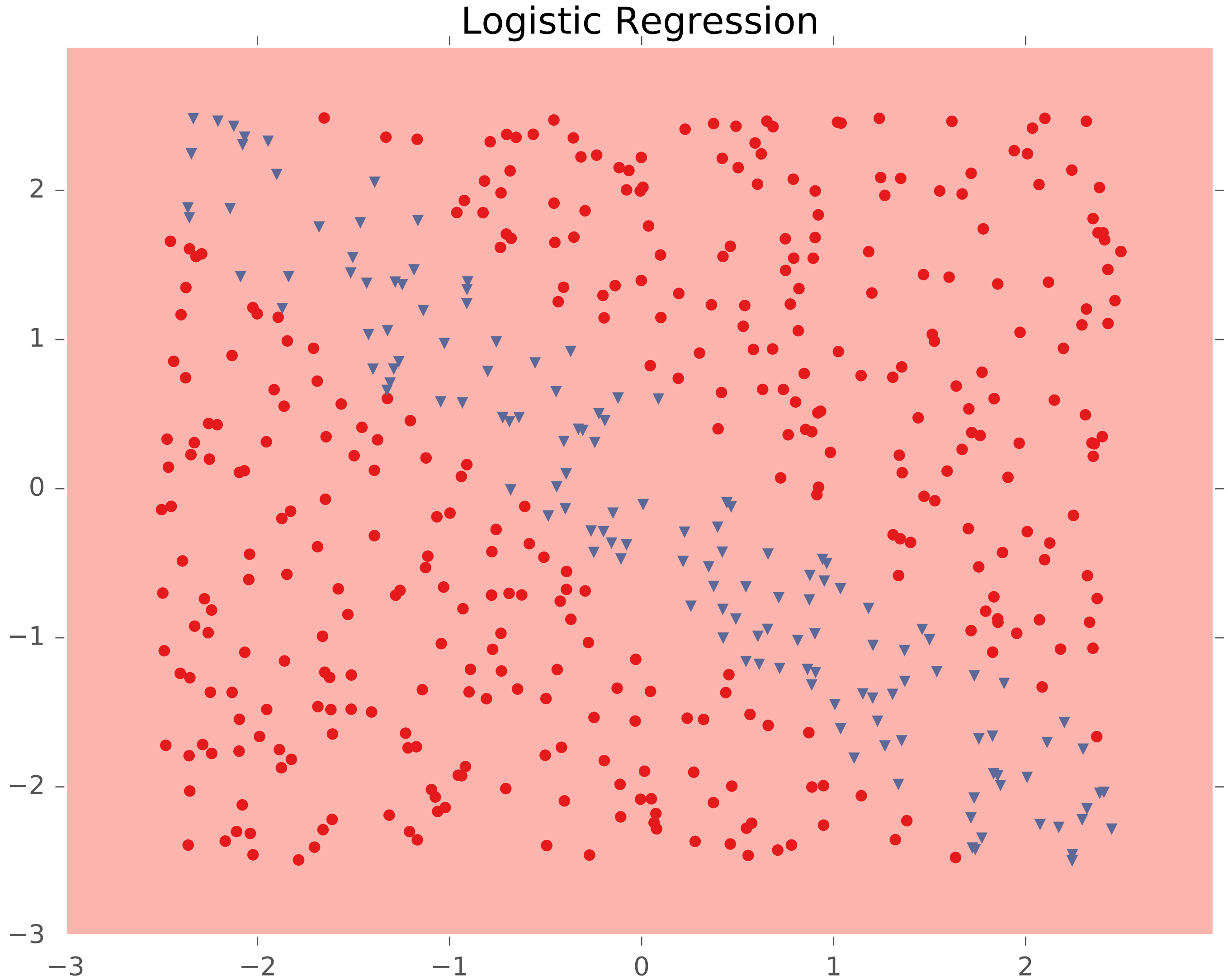

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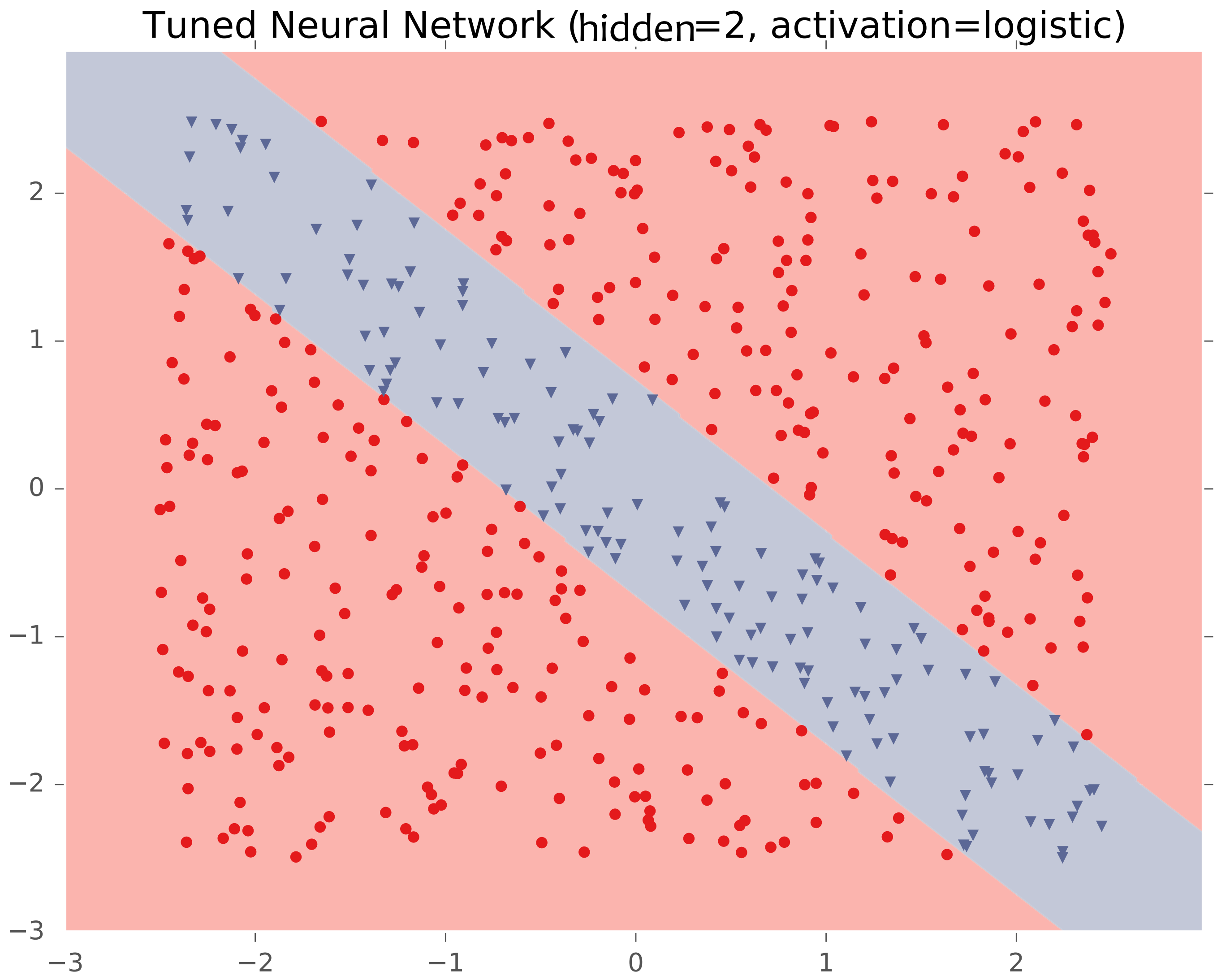

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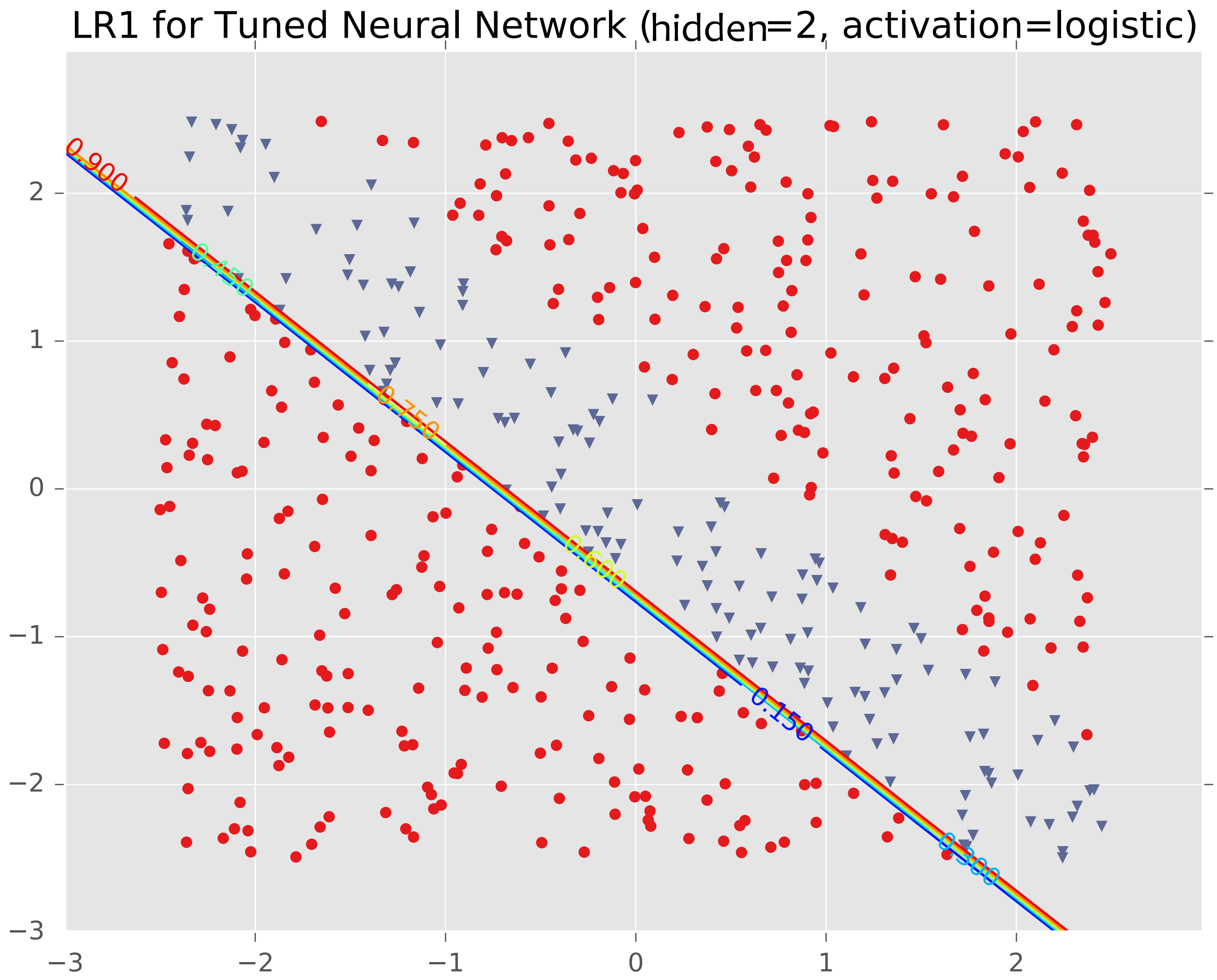

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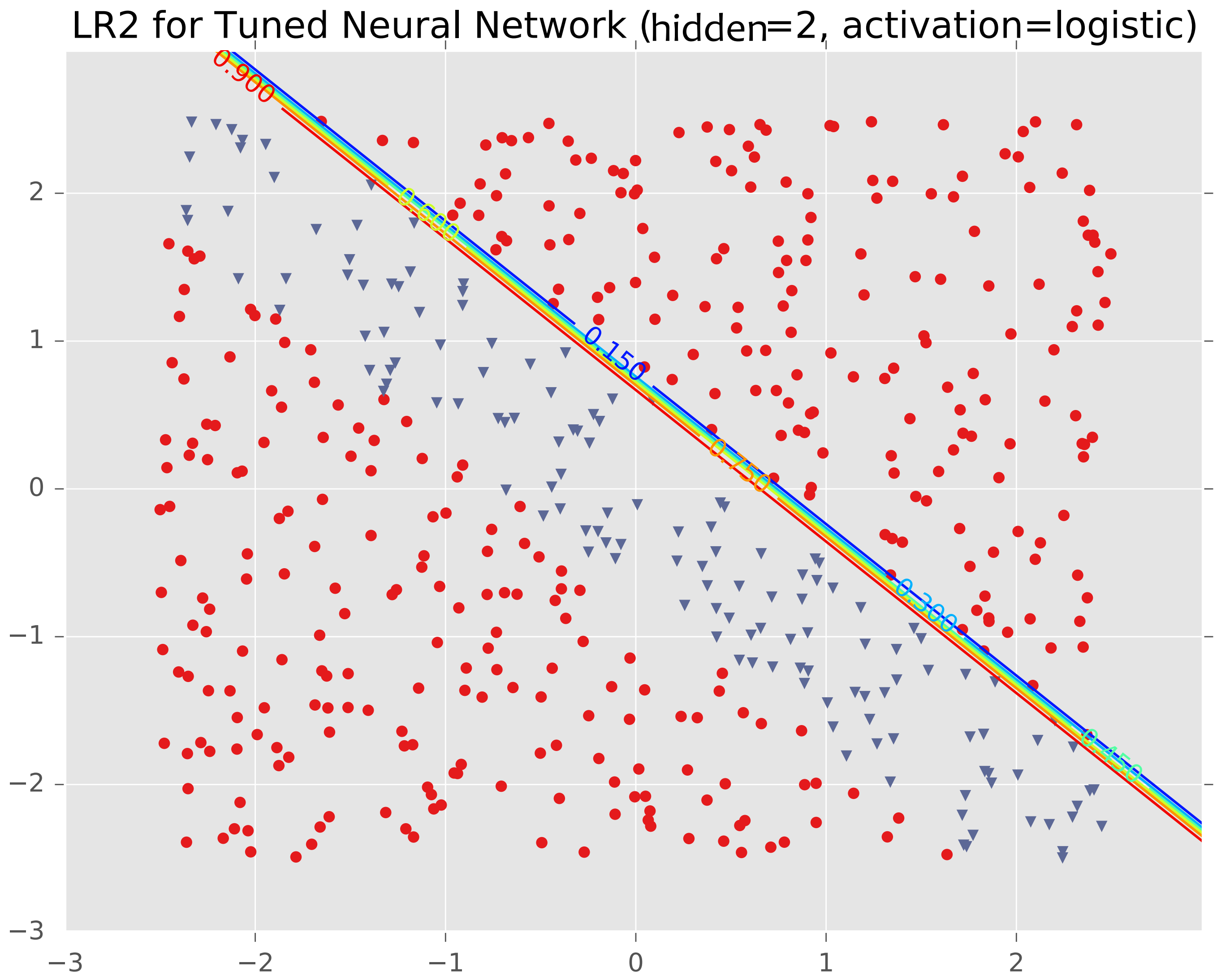

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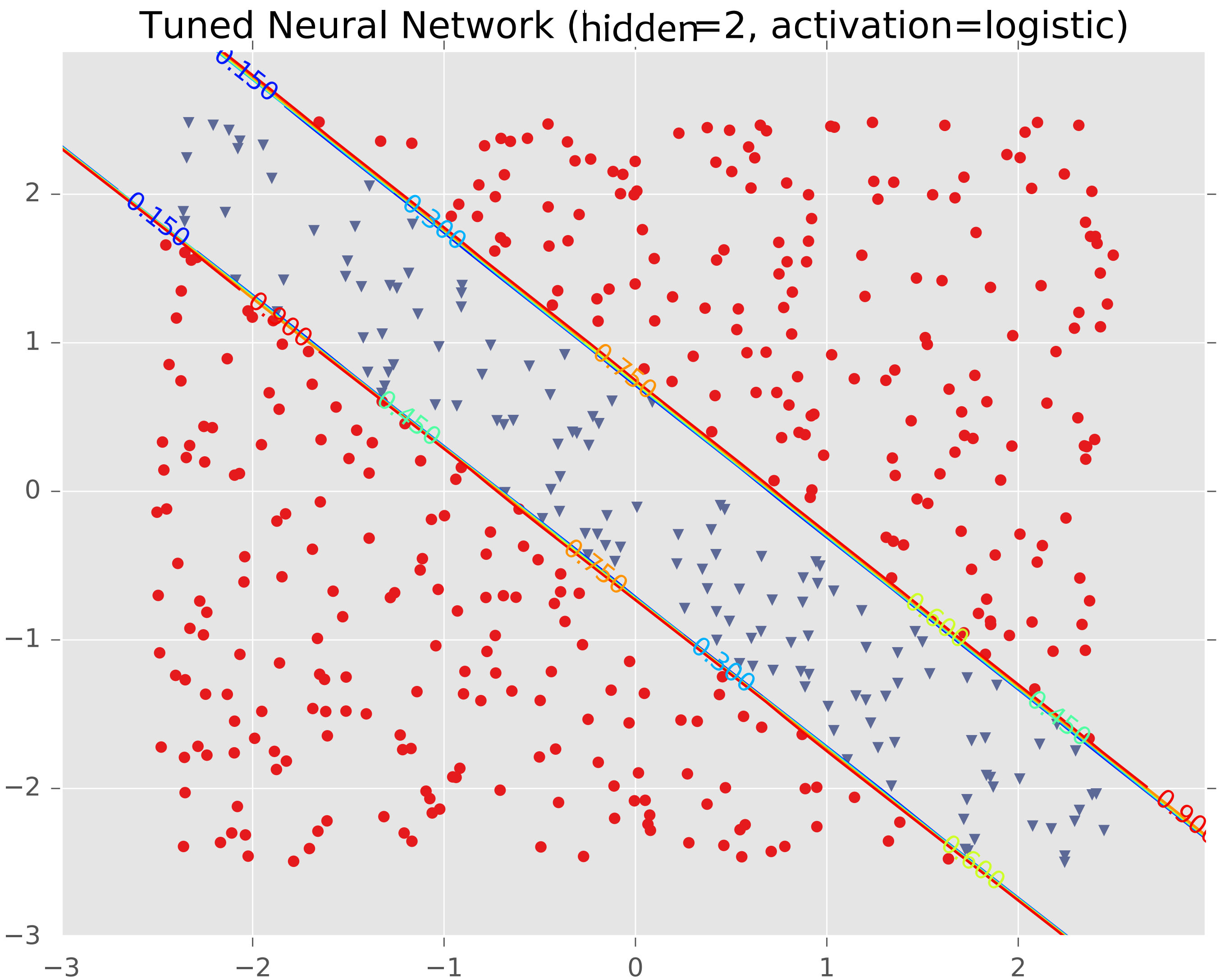
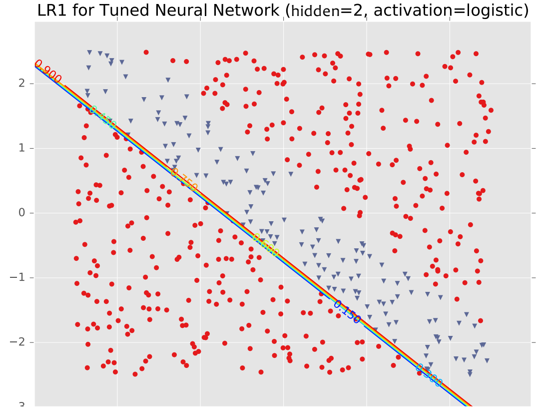
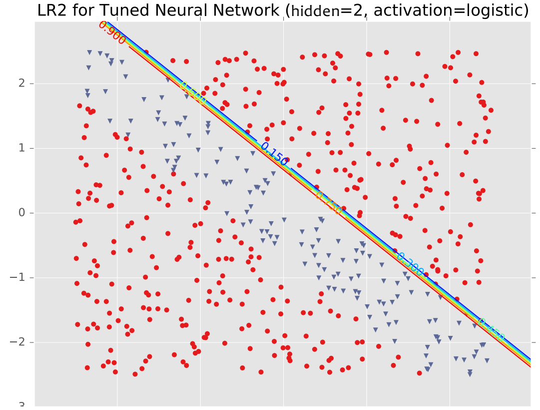
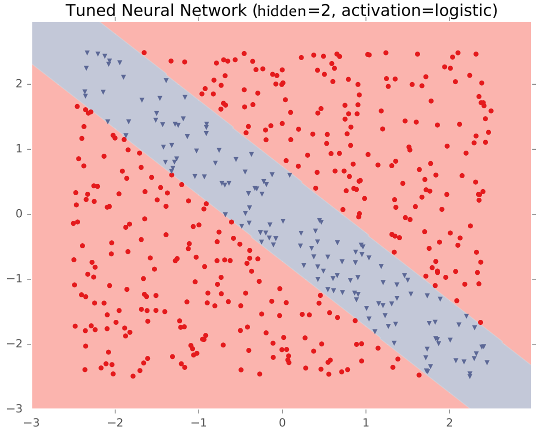
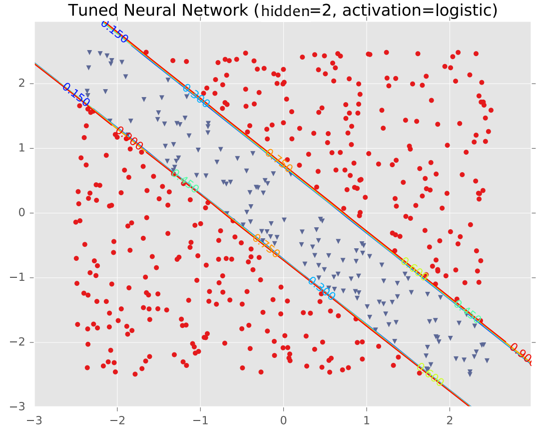


Example #1: Diagonal Band

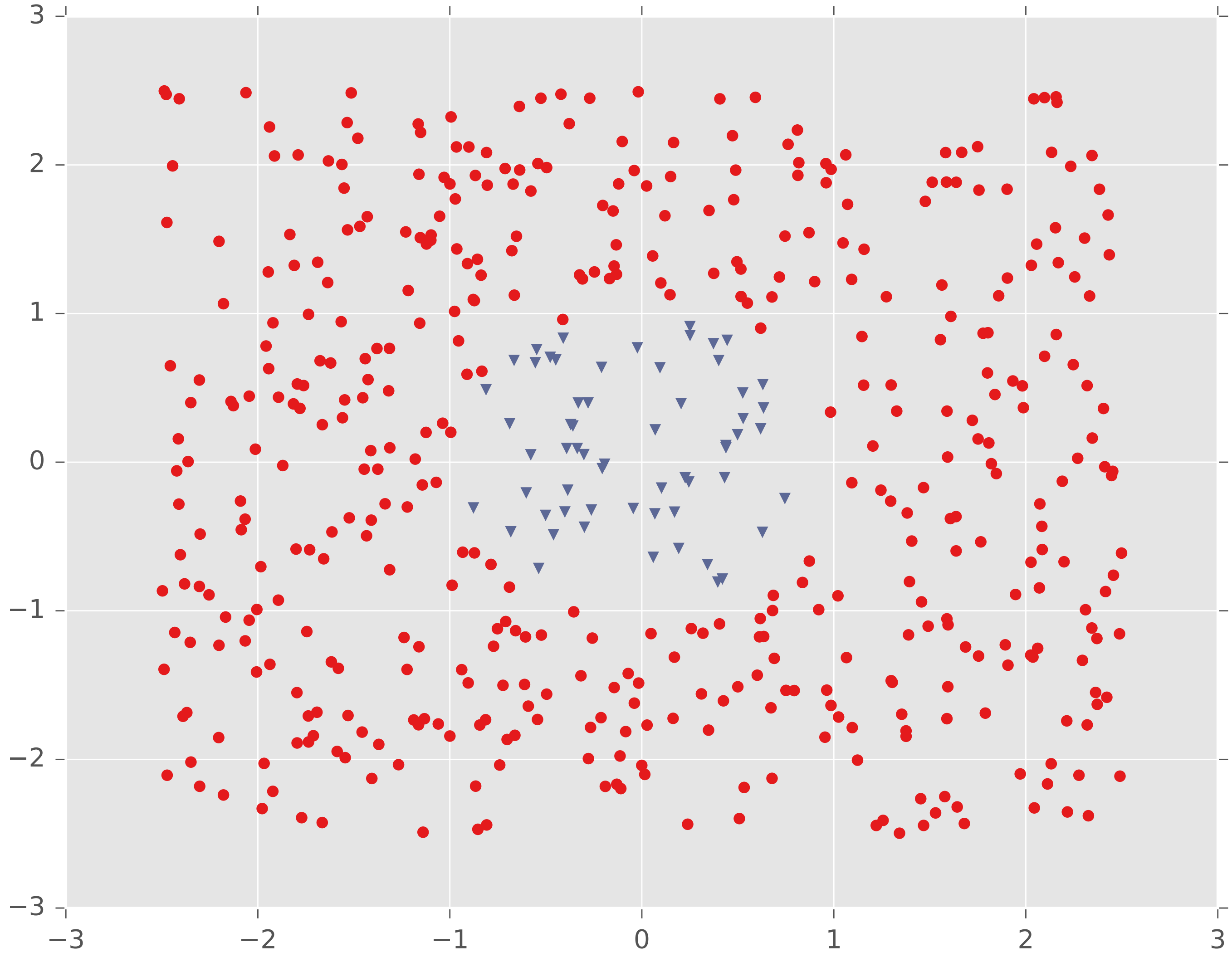








Example #2: One Pocket



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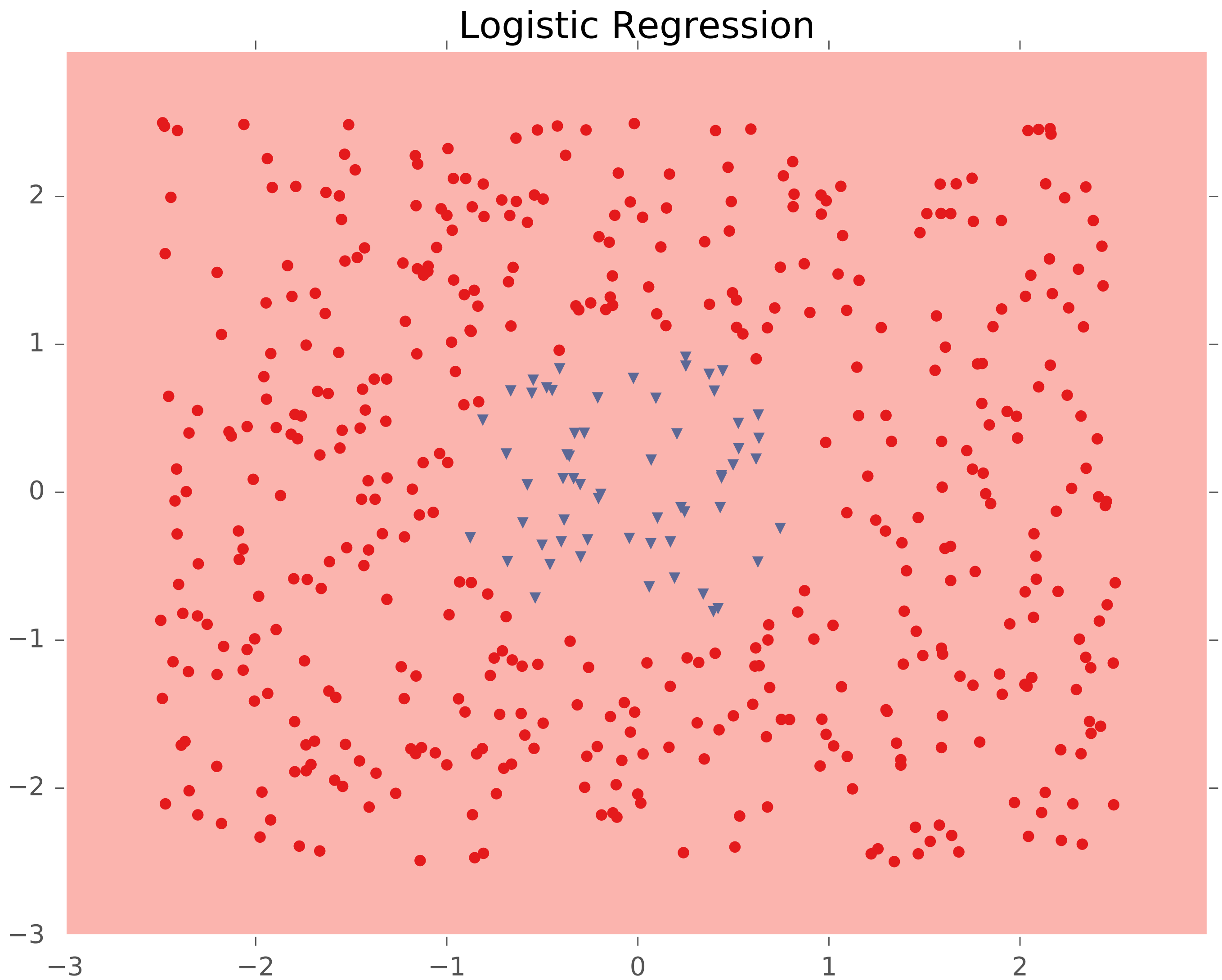

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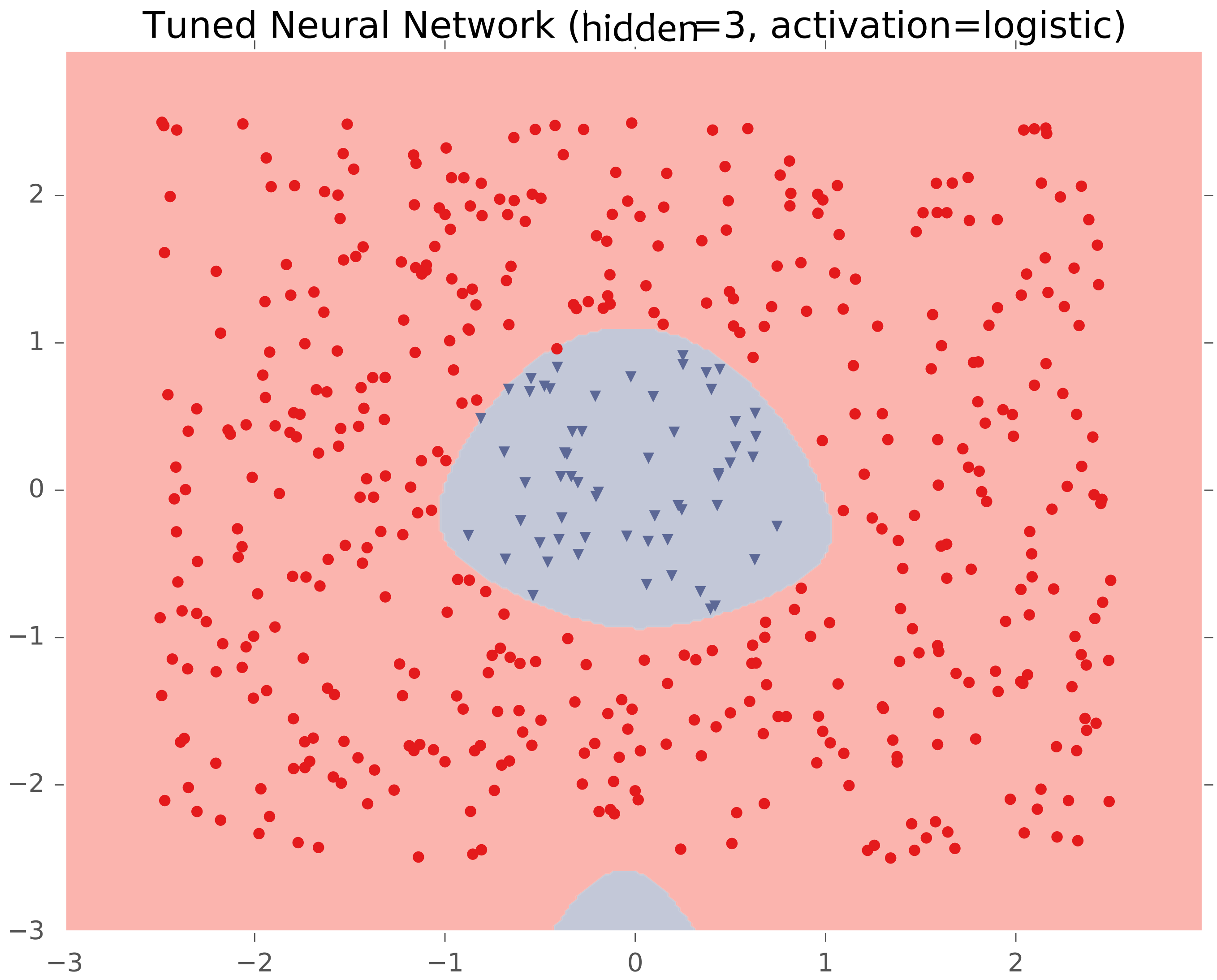

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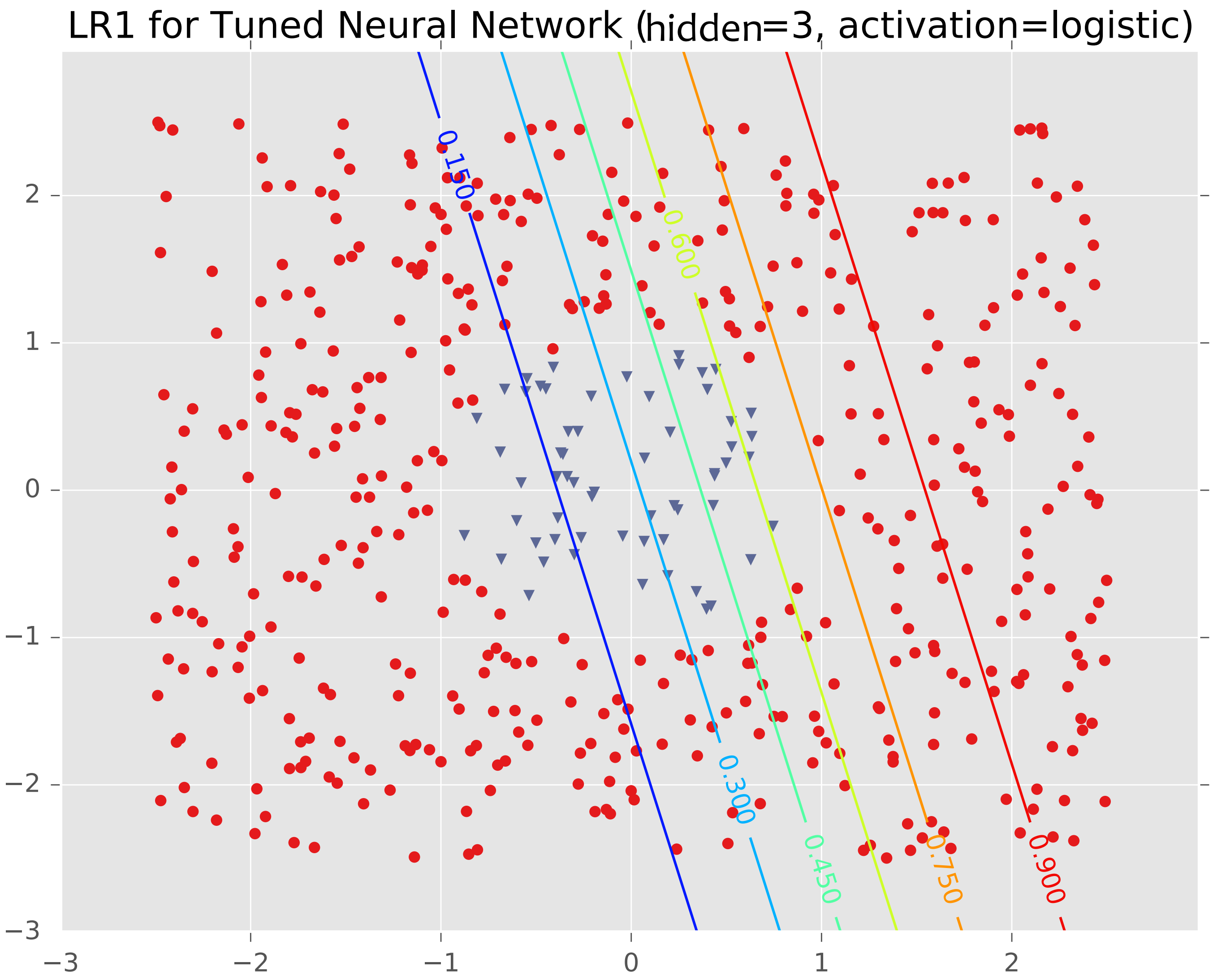

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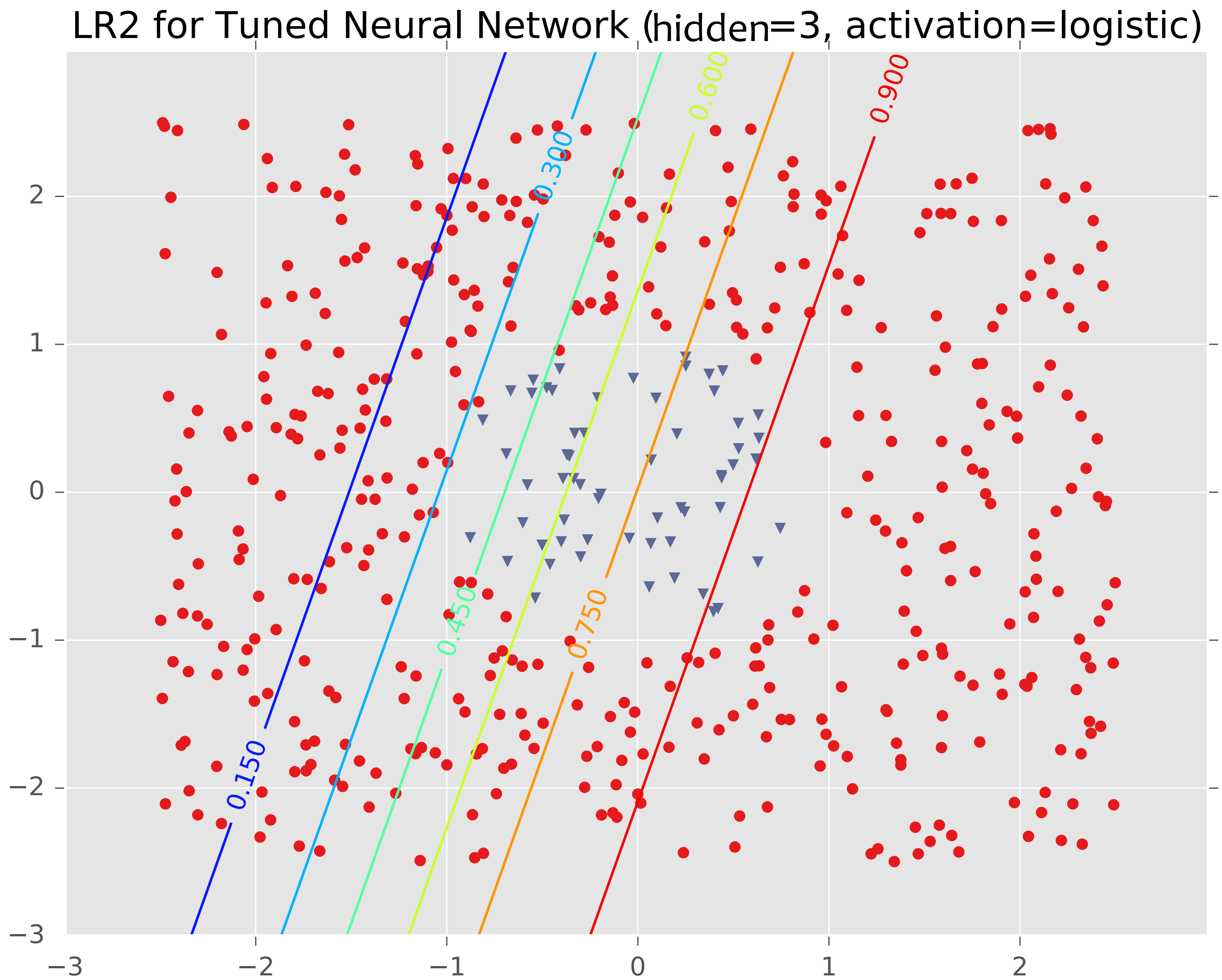

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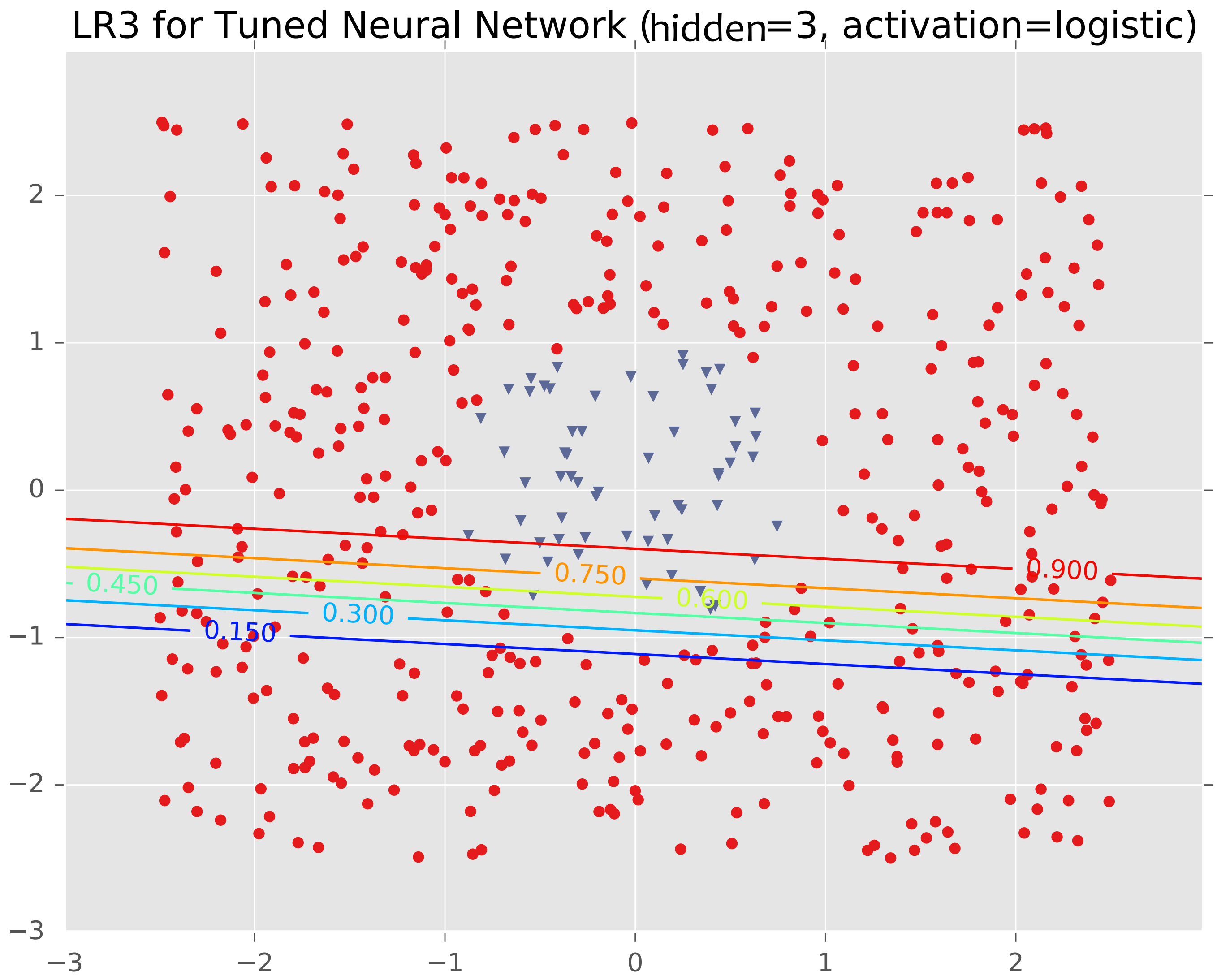

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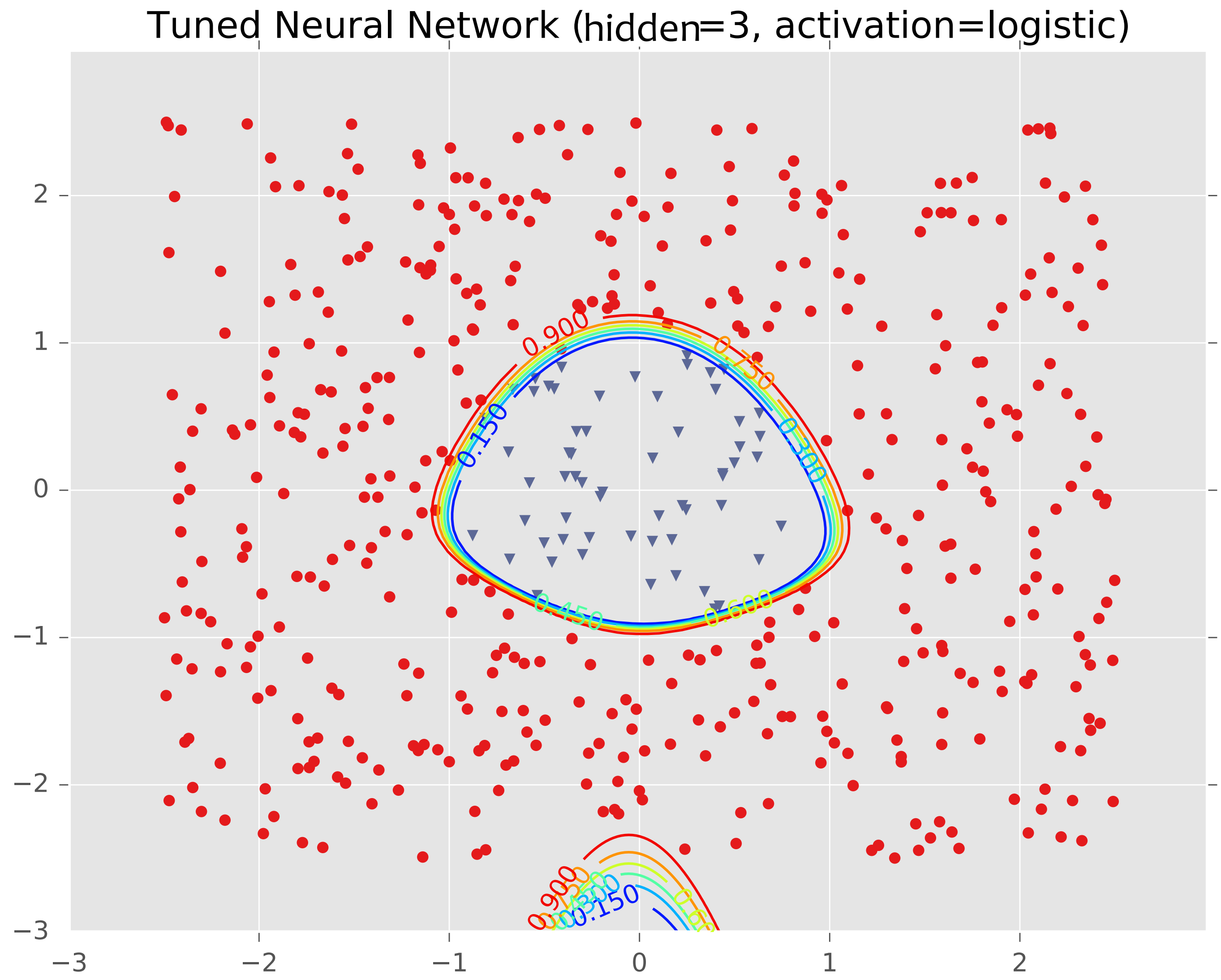

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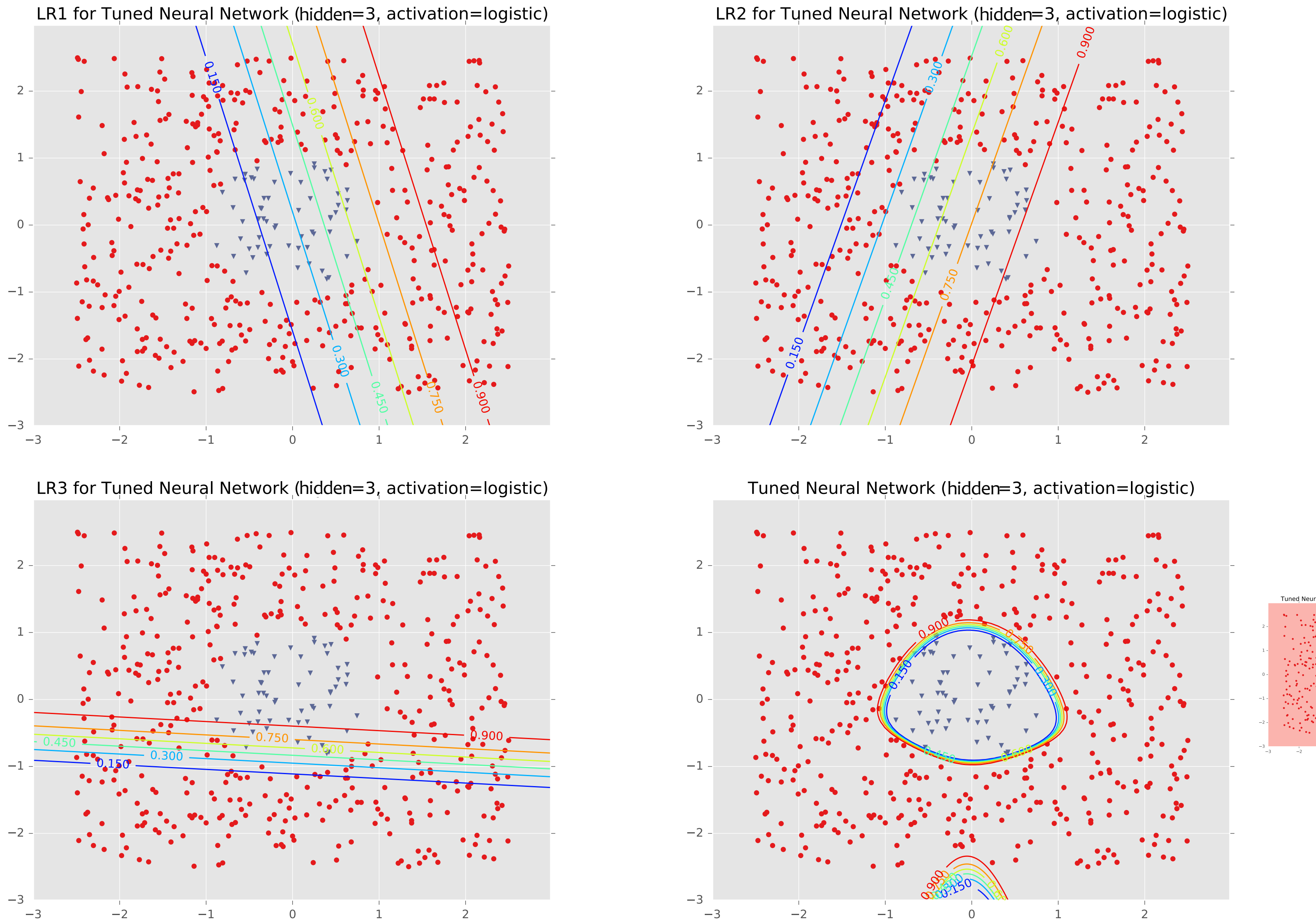
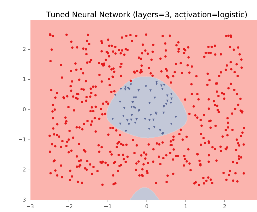
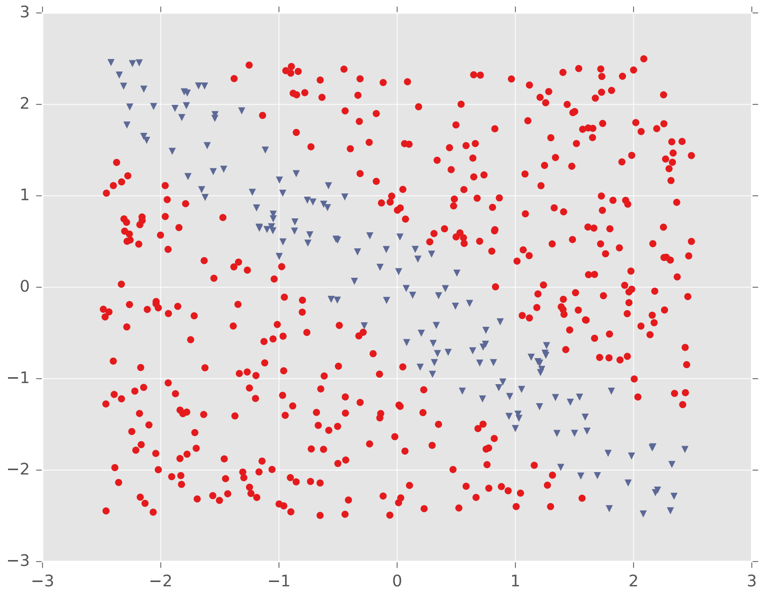




Examples 3 and 4

DECISION BOUNDARY EXAMPLES

Example #1: Diagonal Band



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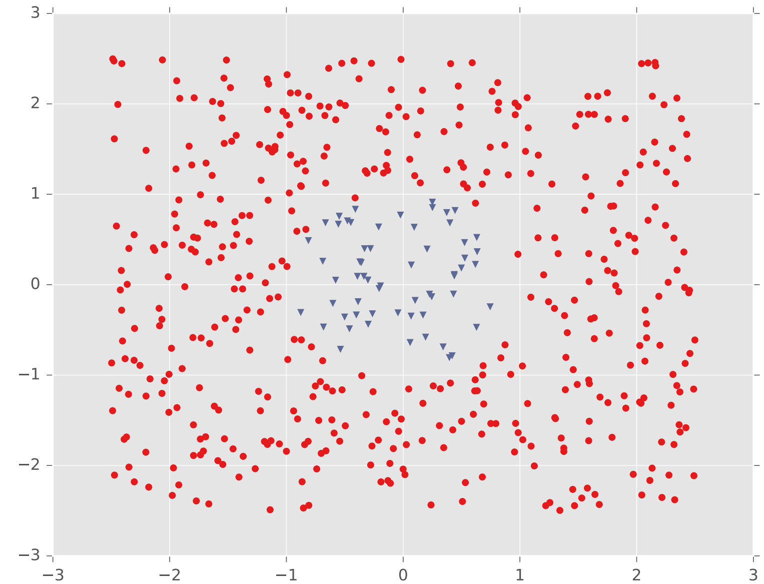
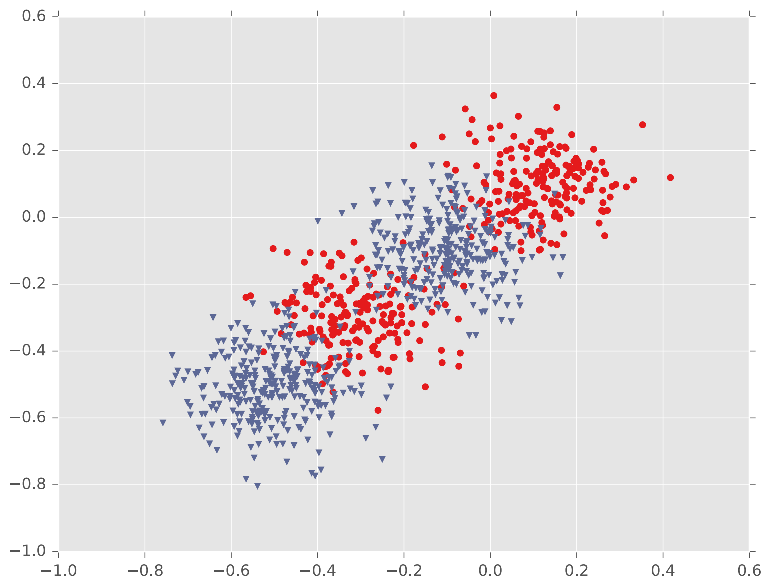
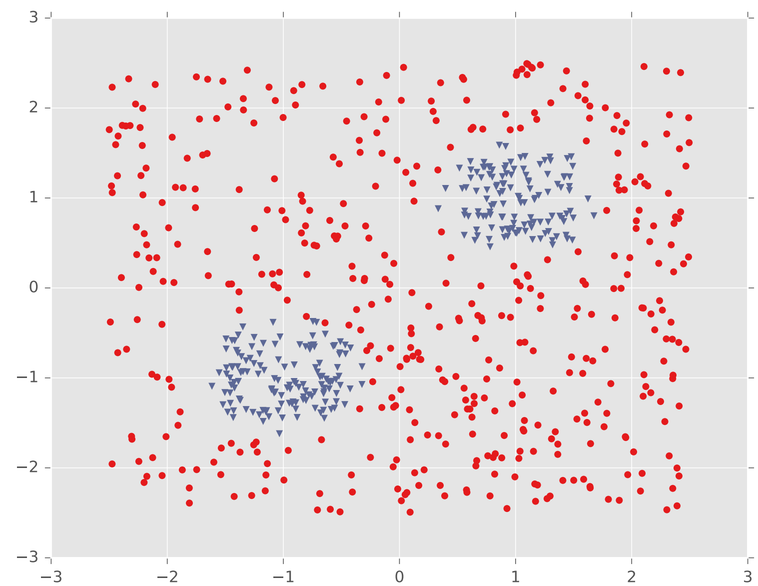


Example #3: Four Gaussians



Example #4: Two Pockets



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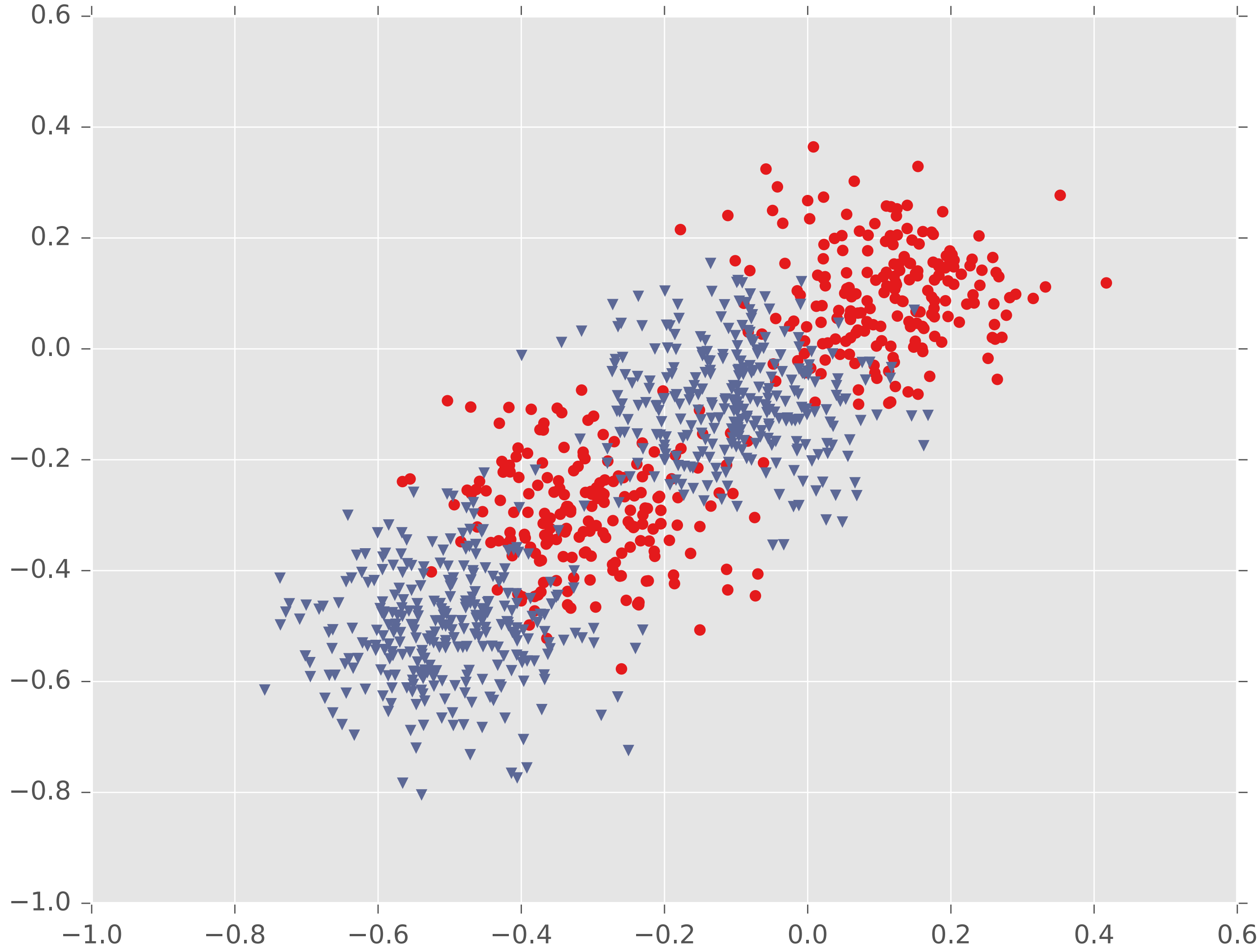

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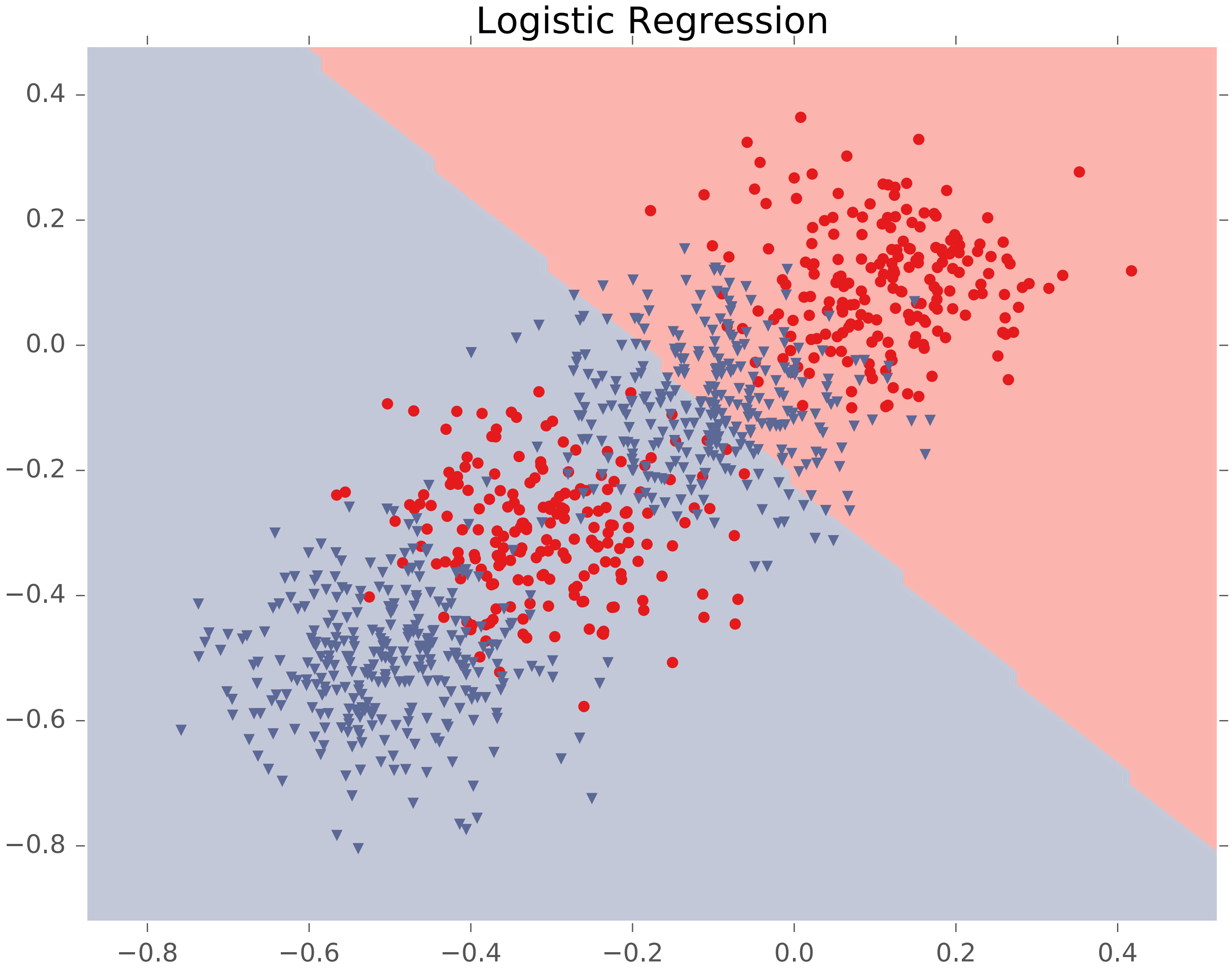

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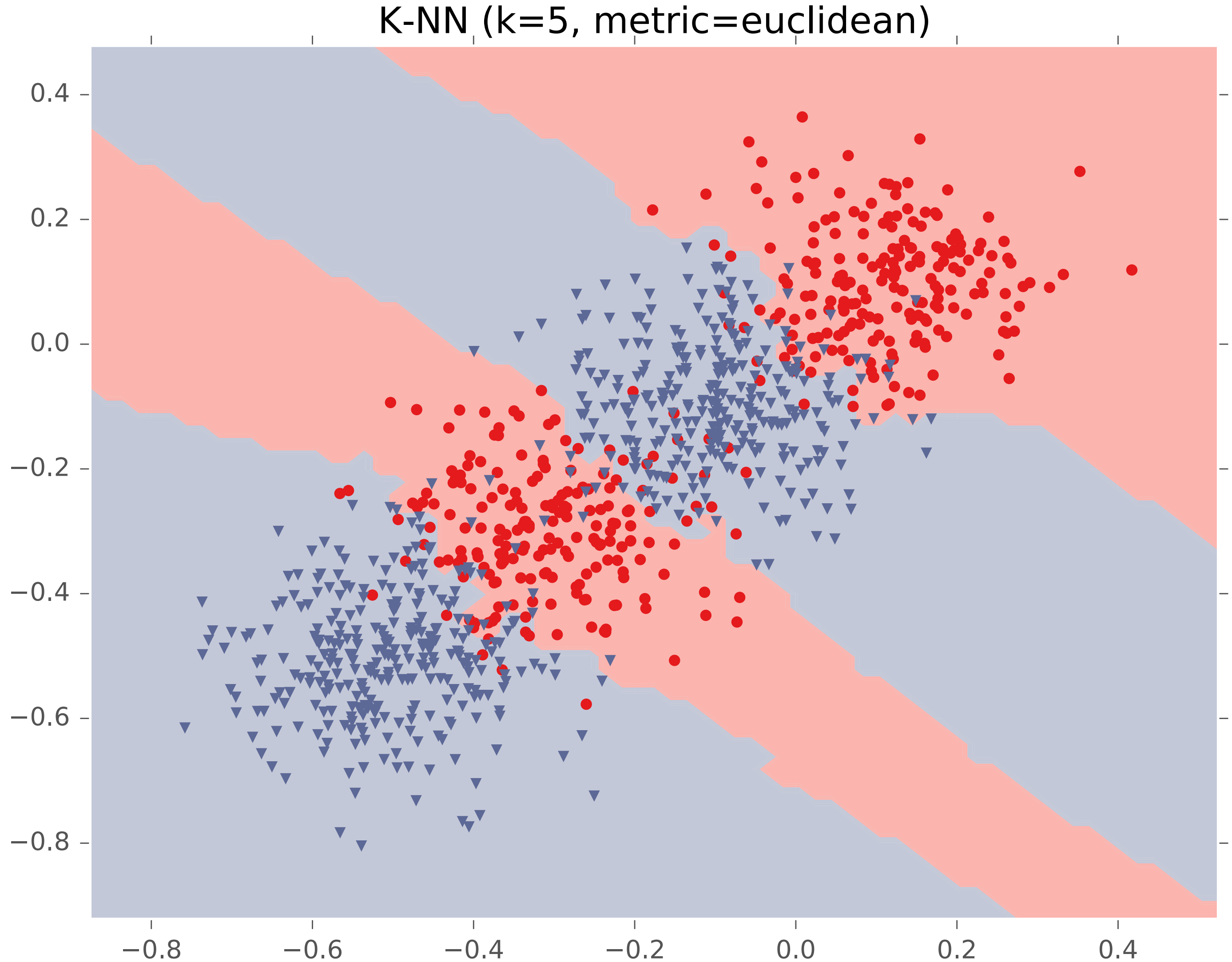

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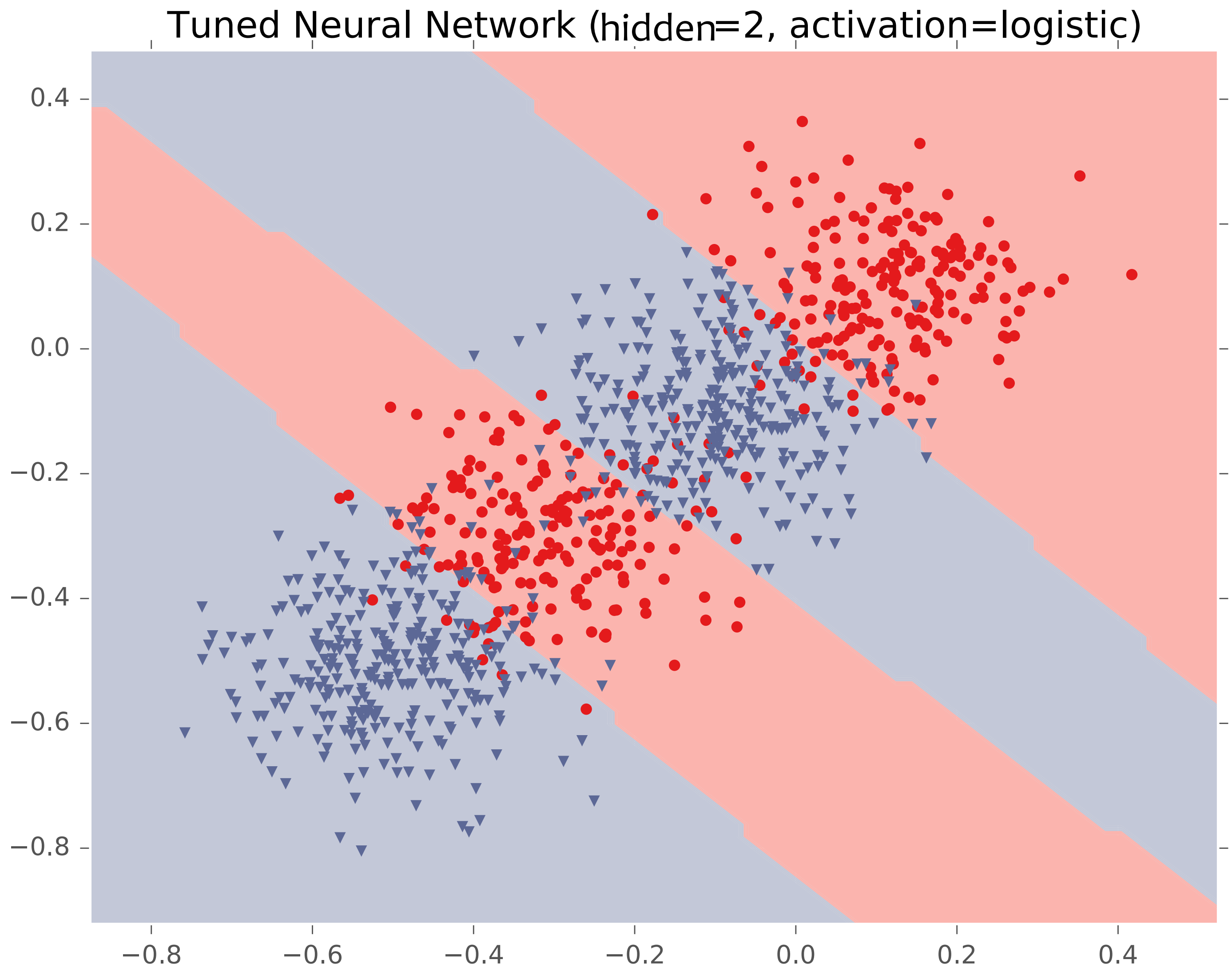

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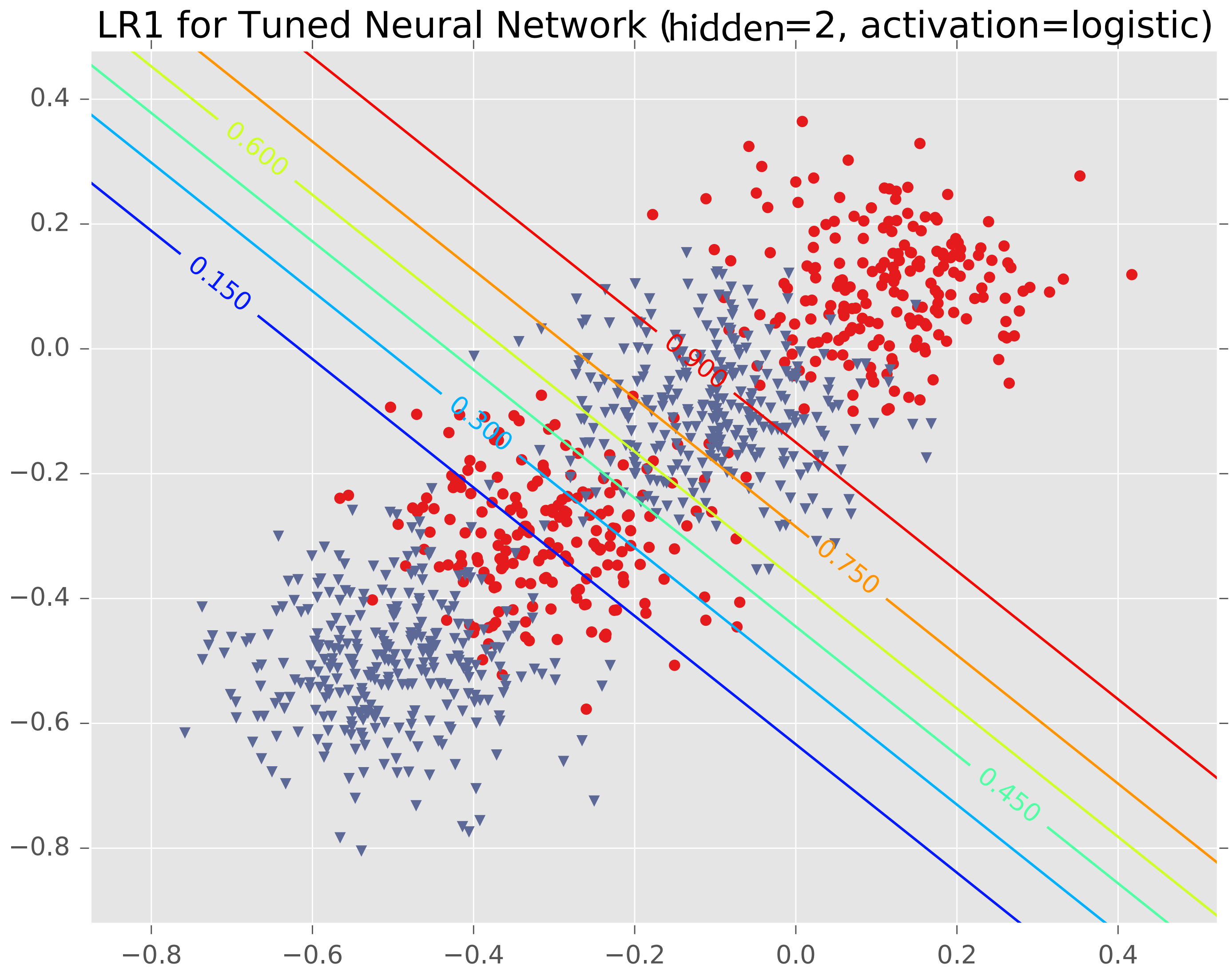

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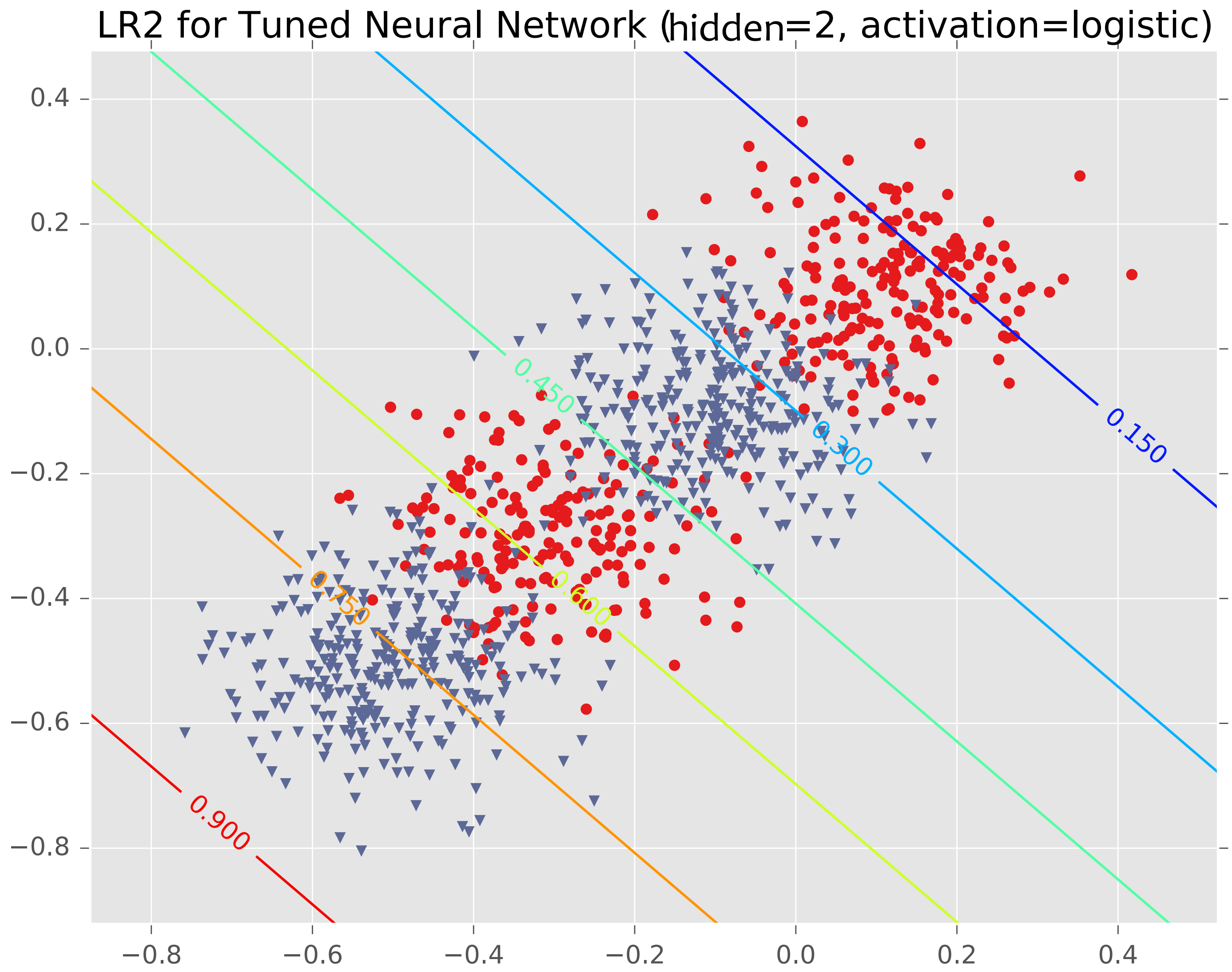

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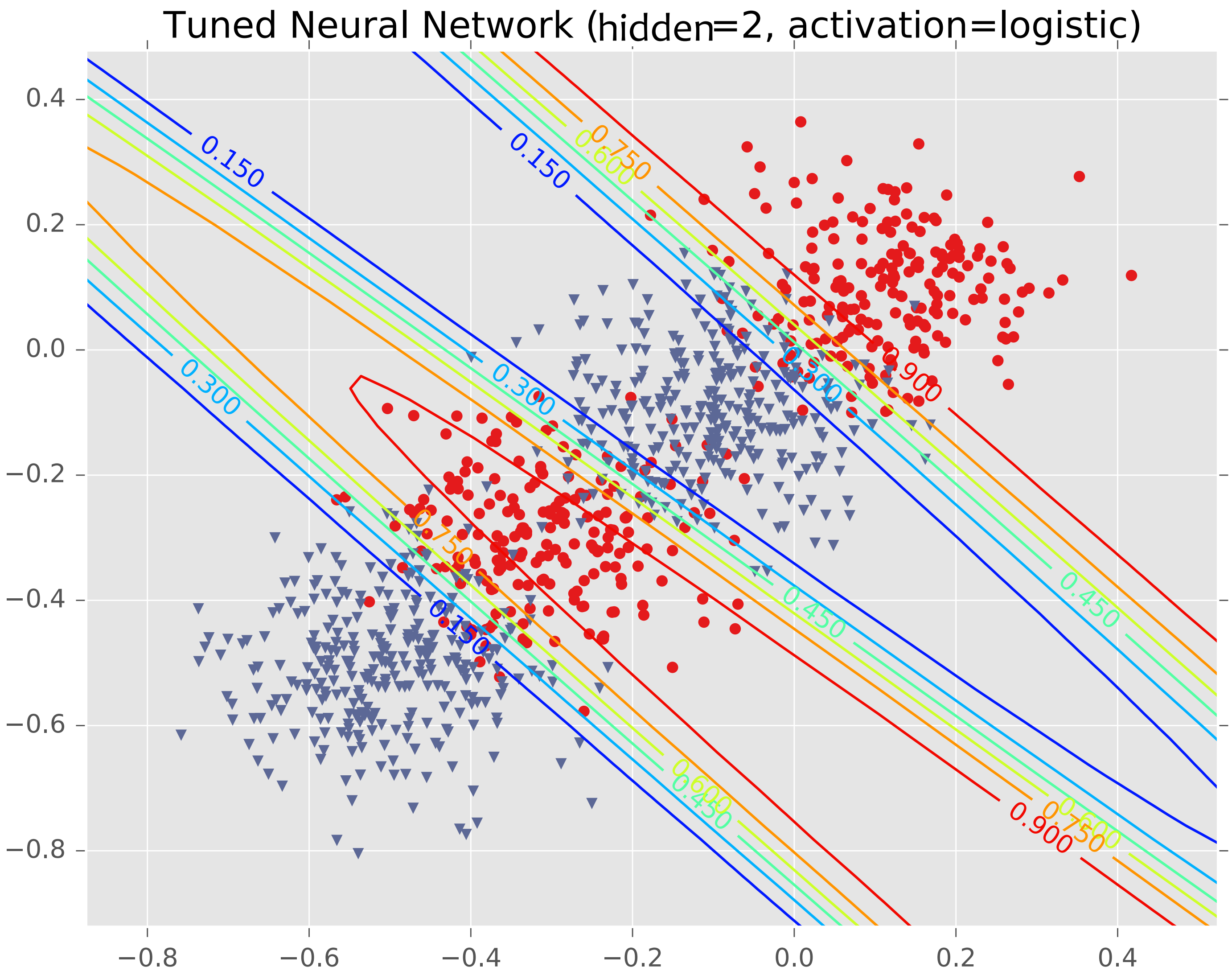
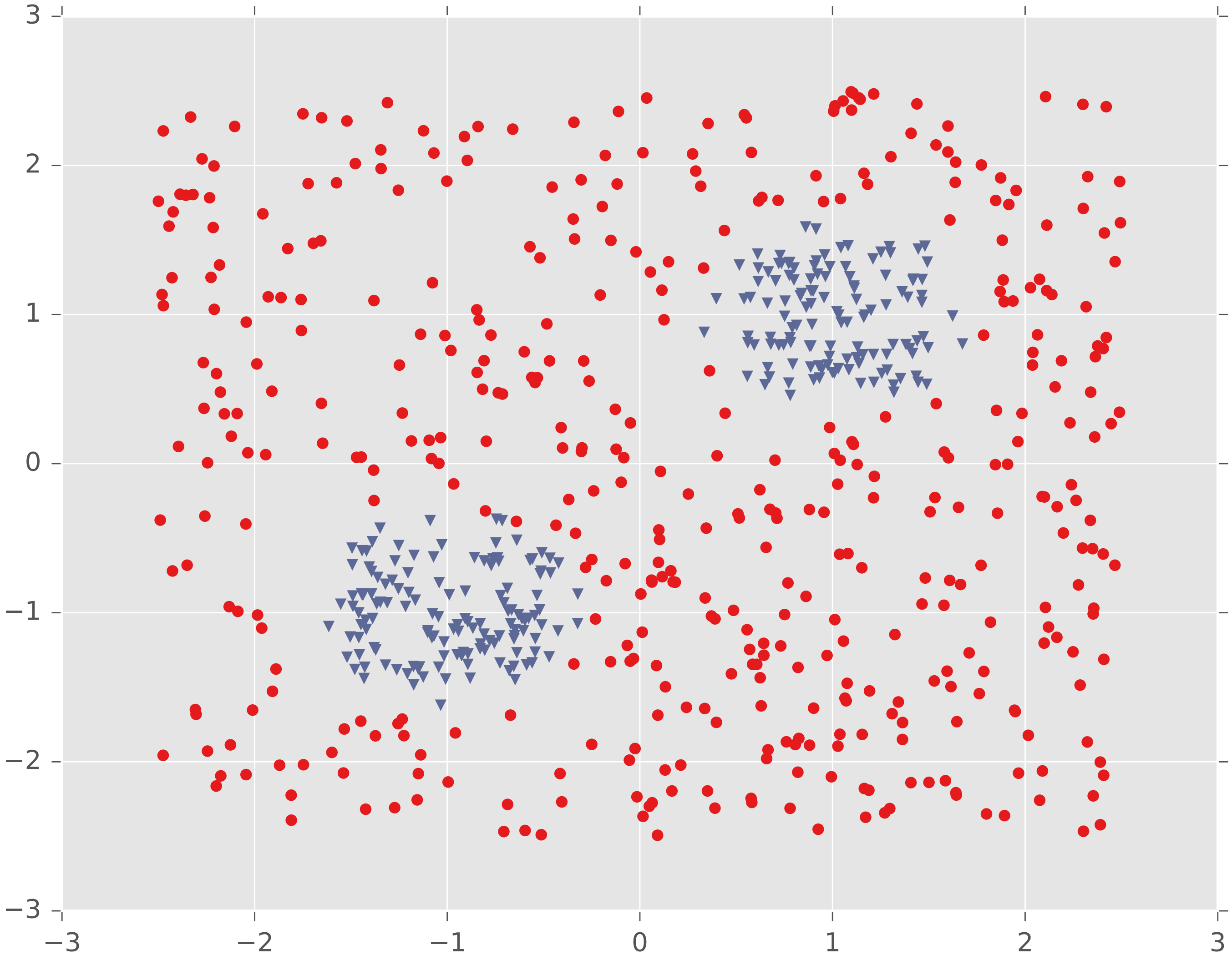
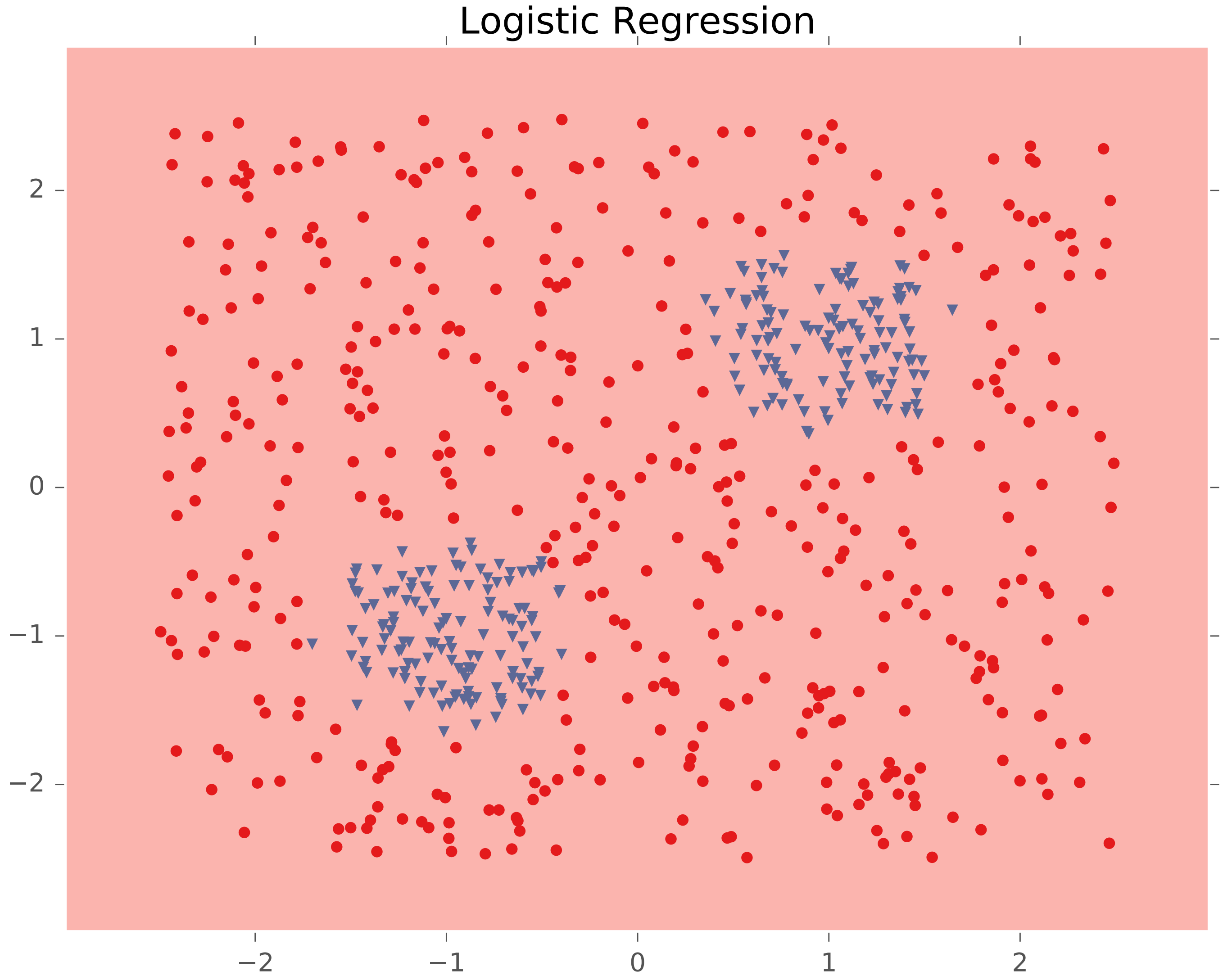


Example #4: Two Pockets



Example #4: Two Pockets



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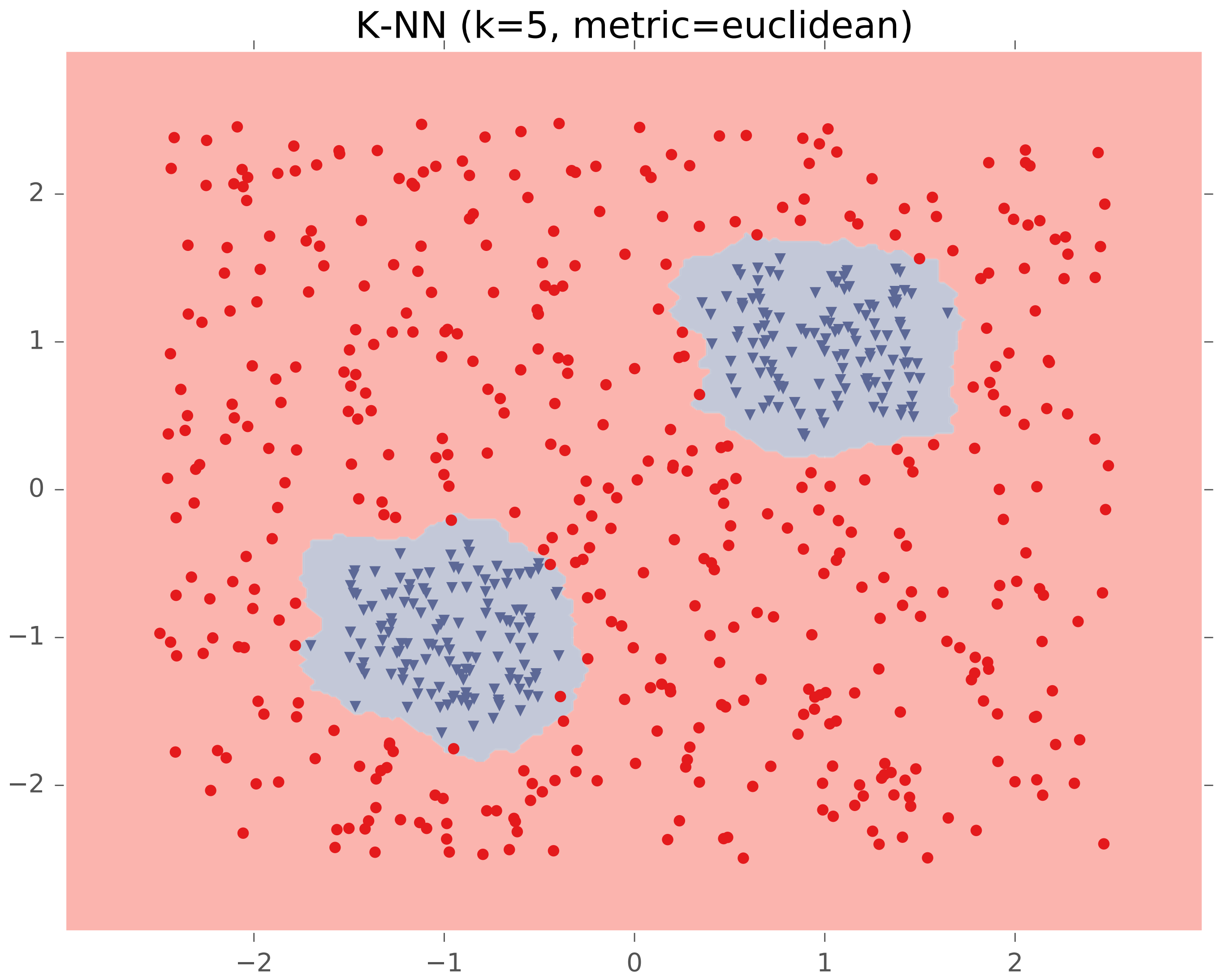

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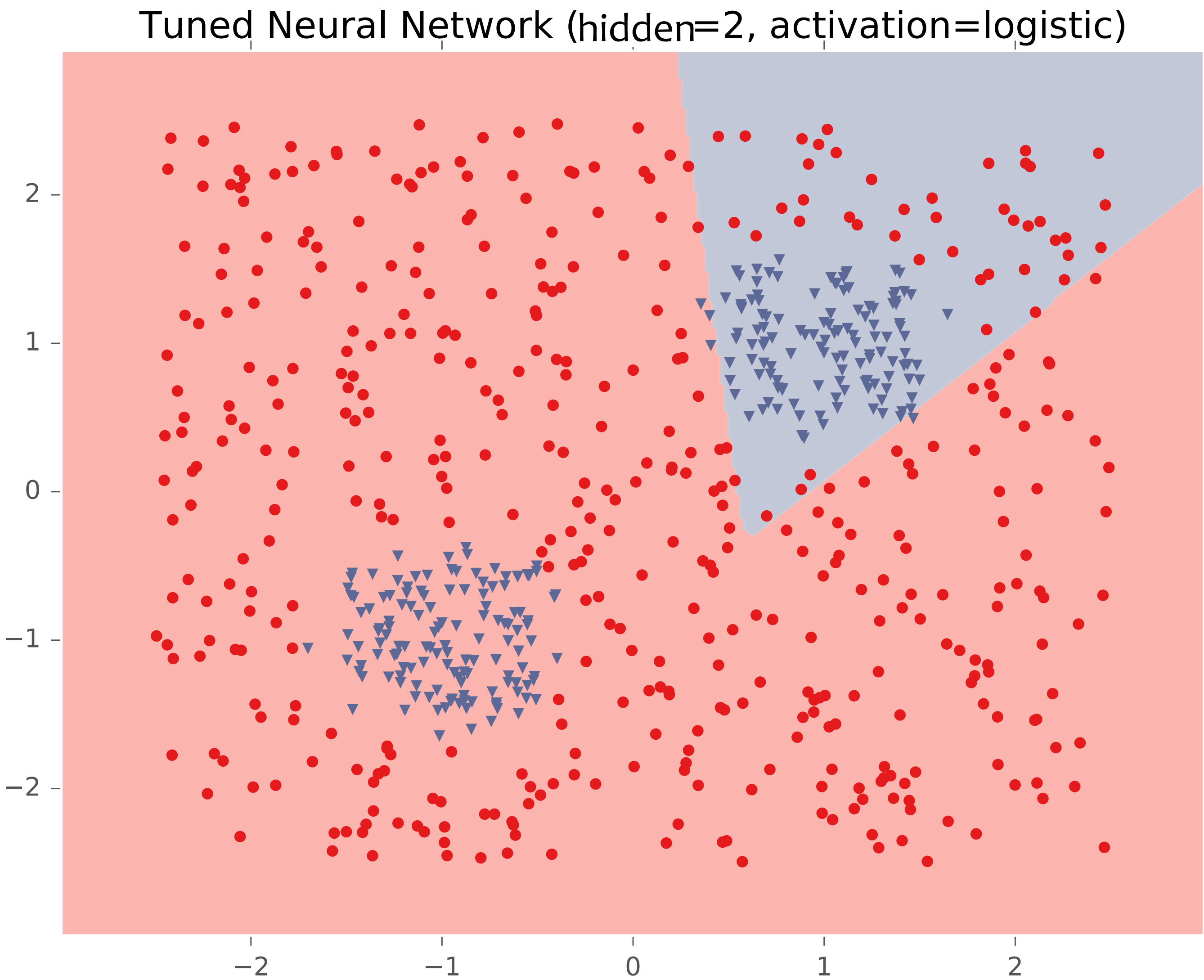

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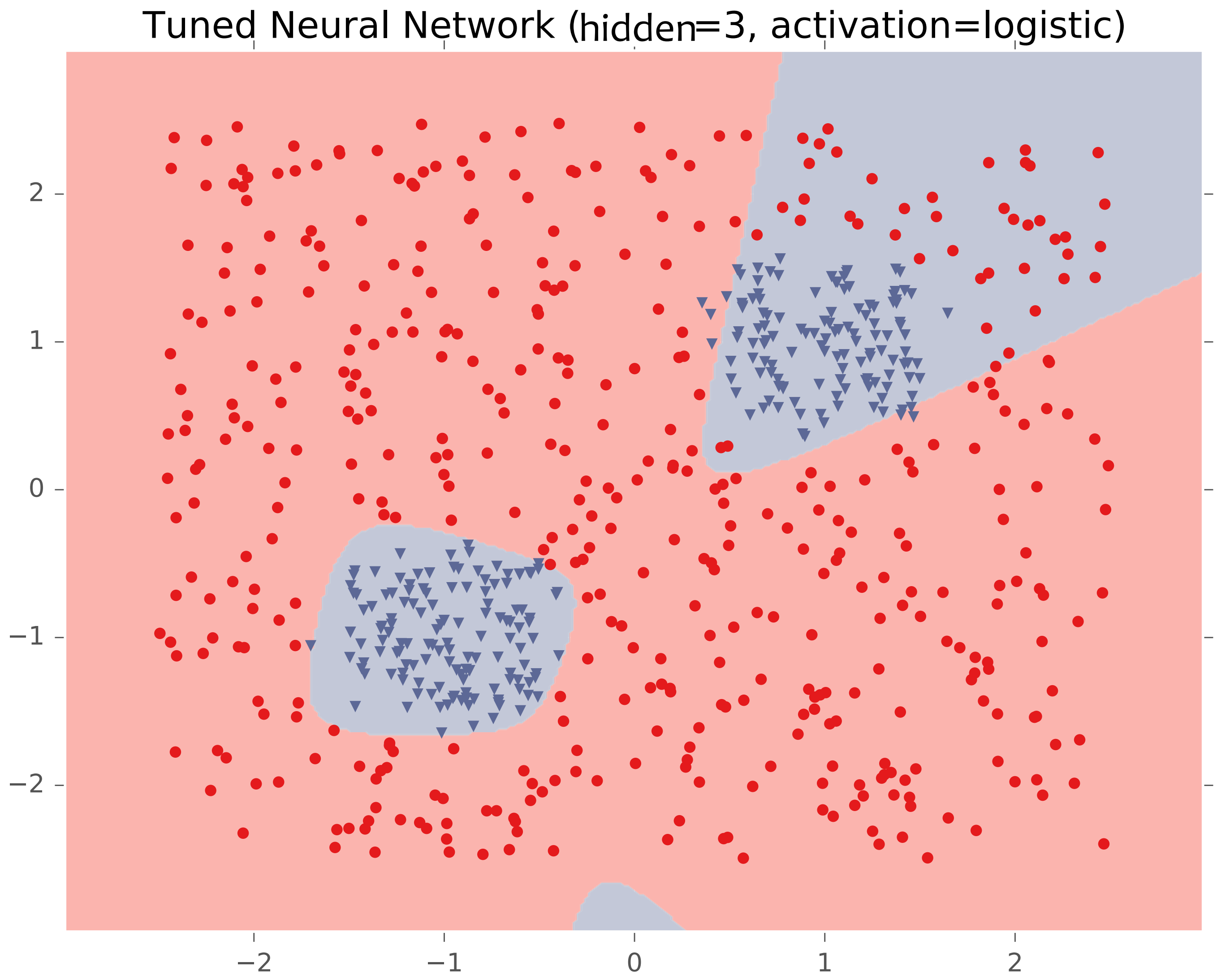

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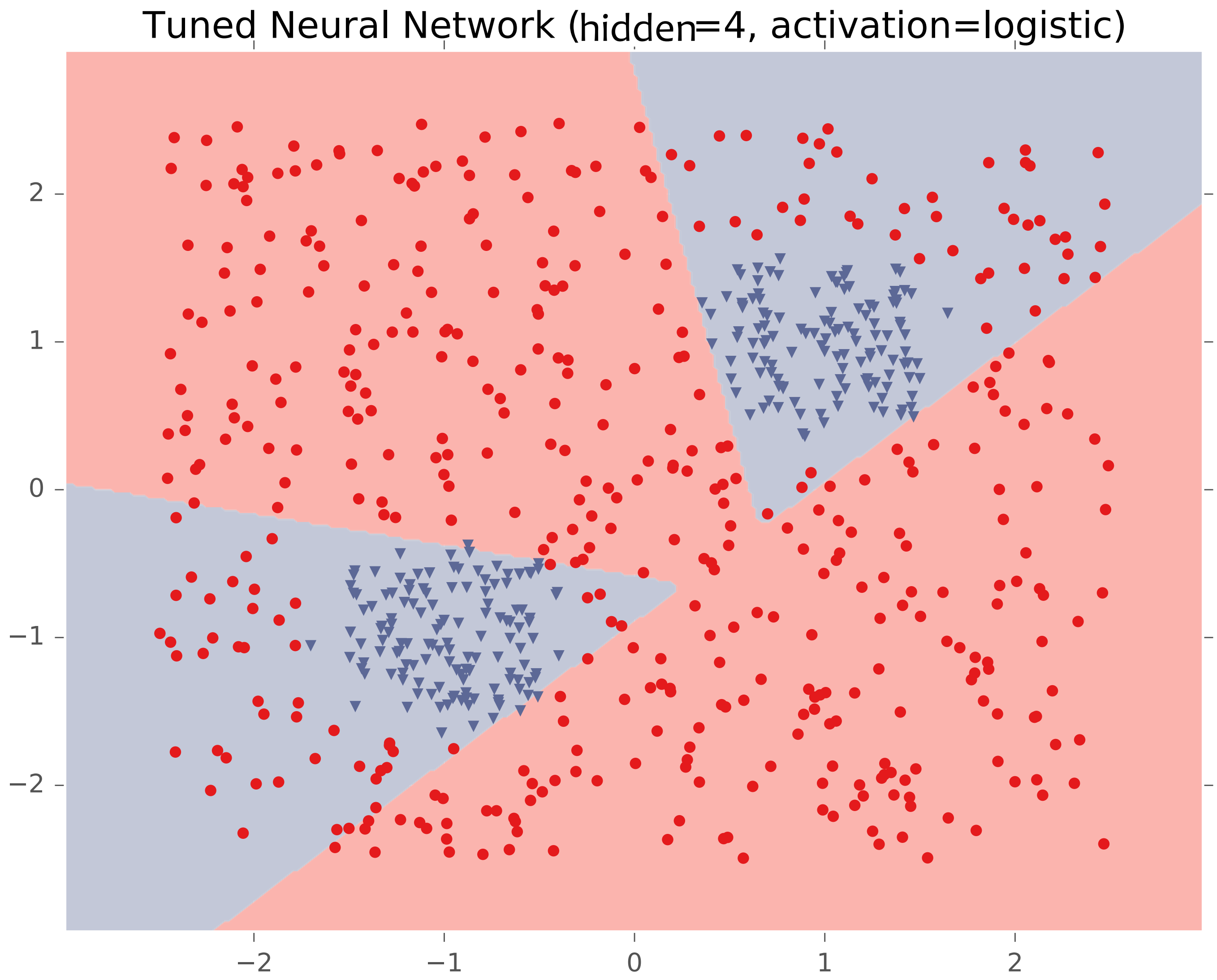

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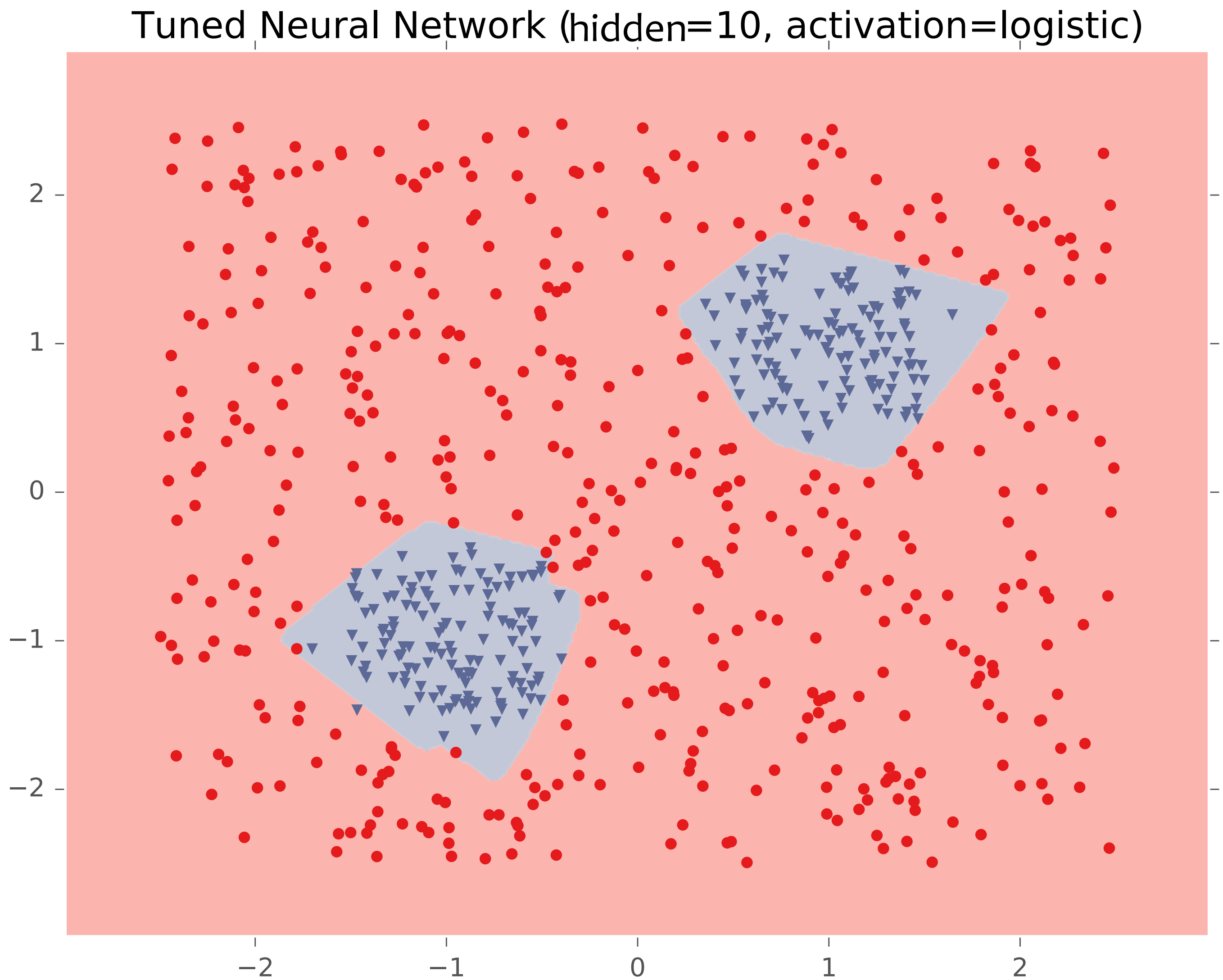
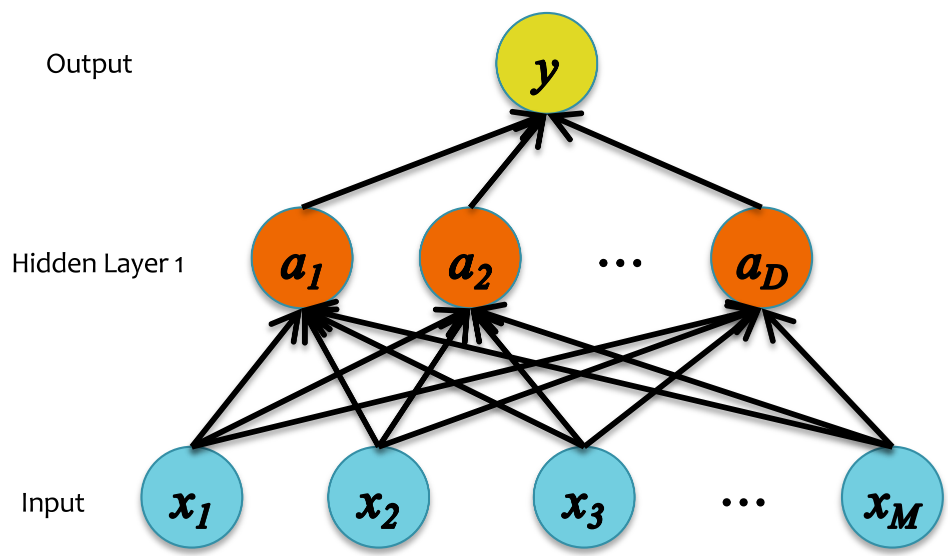


BUILDING DEEPER NETWORKS

Deeper Networks

Q: How many layers should we use?



Deeper Networks

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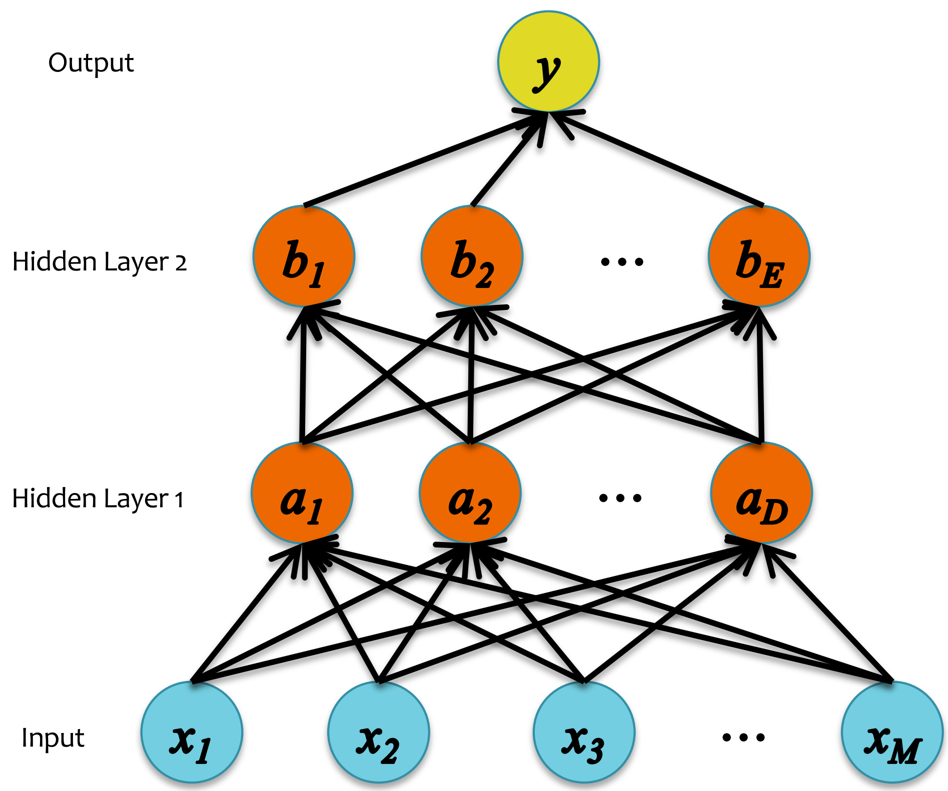

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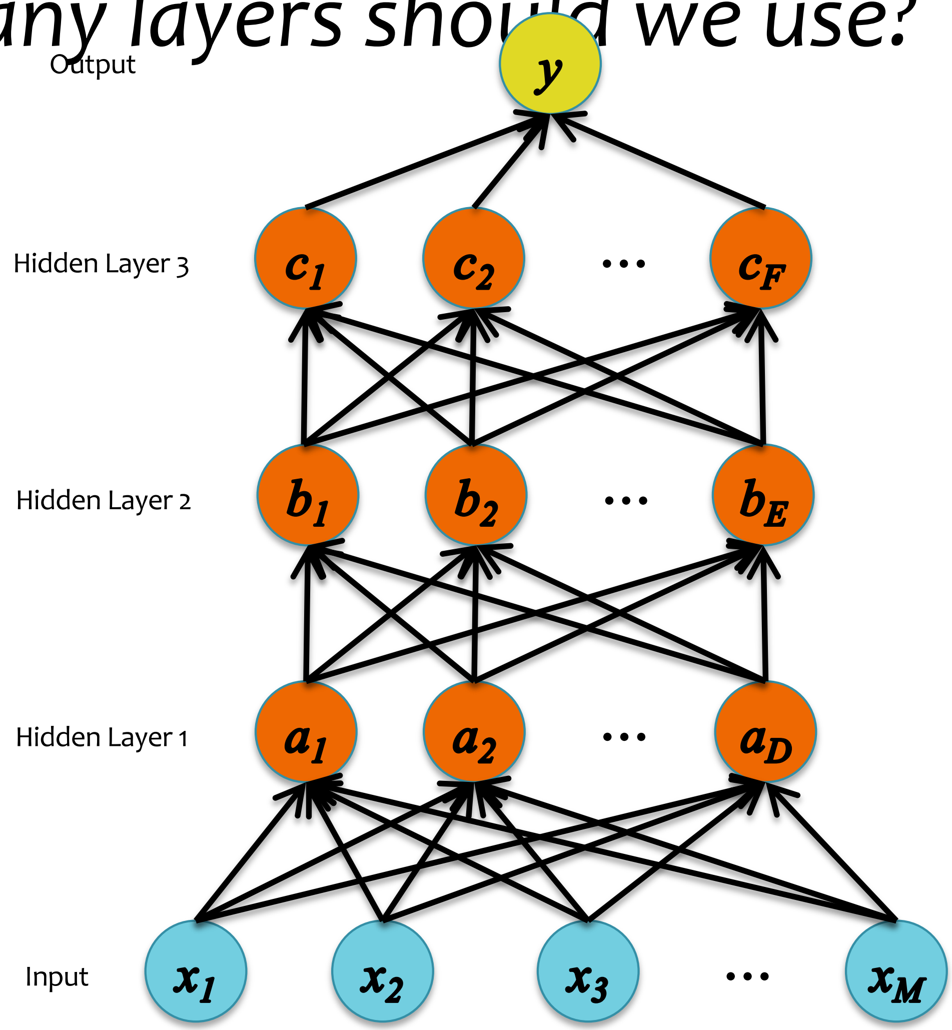


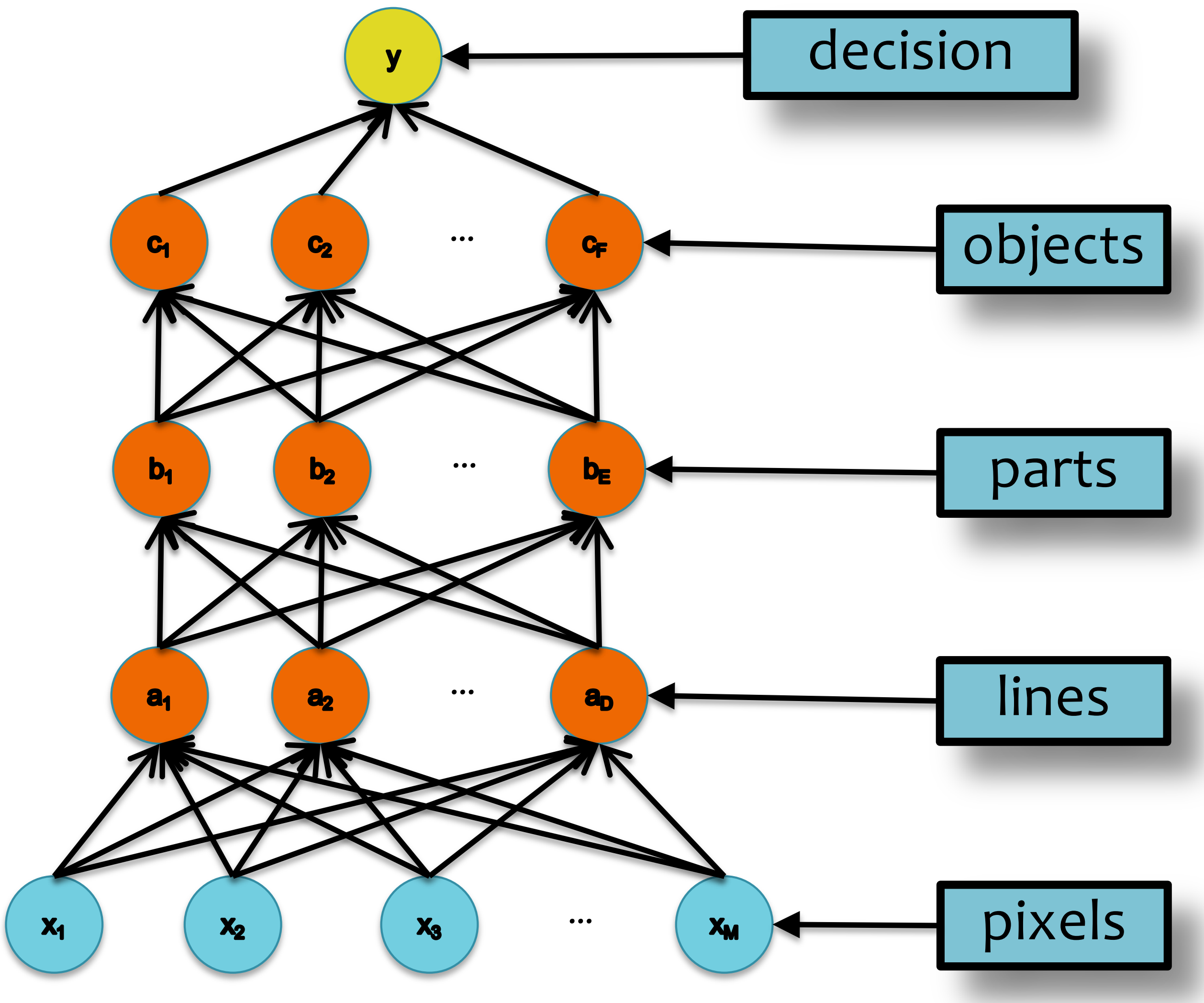
Deeper Networks

Q: How many layers should we use?

- **Theoretical answer:**
  - A neural network with 1 hidden layer is a **universal function approximator**
  - Cybenko (1989): For any continuous function $g(\mathbf{x})$, there exists a 1-hidden-layer neural net $h_\theta(\mathbf{x})$ s.t. $| h_\theta(\mathbf{x}) - g(\mathbf{x}) | < \epsilon$ for all $\mathbf{x}$, assuming sigmoid activation functions
- **Empirical answer:**
  - Before 2006: "Deep networks (e.g. 3 or more hidden layers) are too hard to train"
  - After 2006: "Deep networks are easier to train than shallow networks (e.g. 2 or fewer layers) for many problems"

    Big caveat: You need to know and use the right tricks.

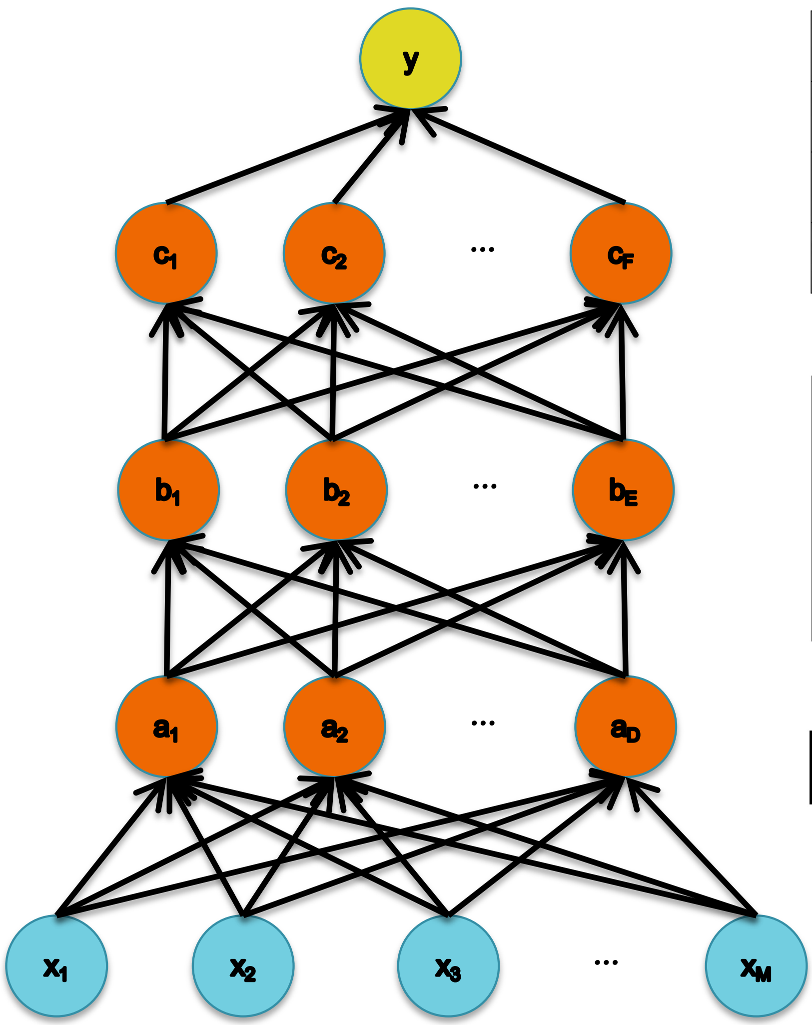
Feature Learning



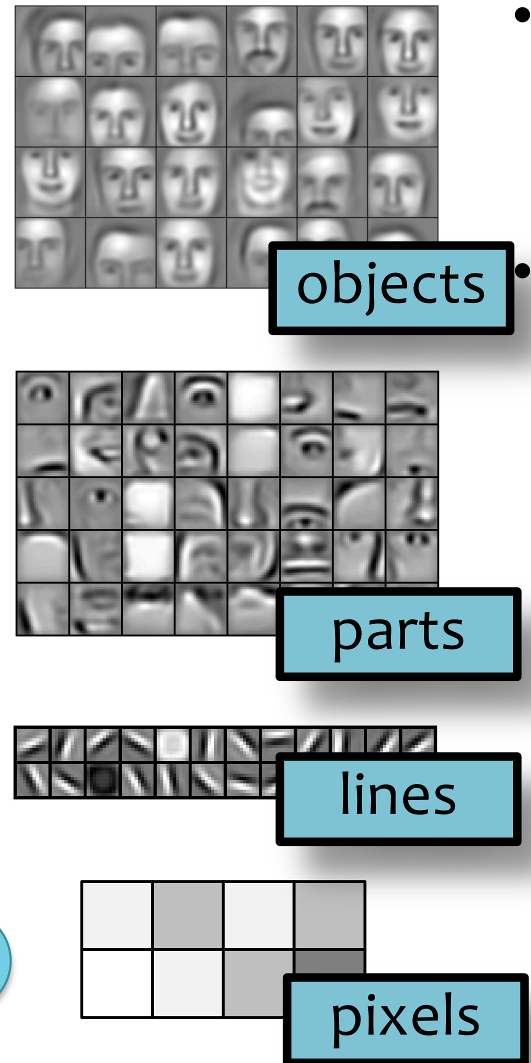
- **Traditional feature engineering:** build up levels of abstraction by hand
- **Deep networks** (e.g. convolution networks): learn the increasingly higher levels of abstraction from data
  - each layer is a learned feature representation
  - sophistication increases in higher layers

Figures from Lee et al. (ICML 2009)

Feature Learning



CBDN on Faces



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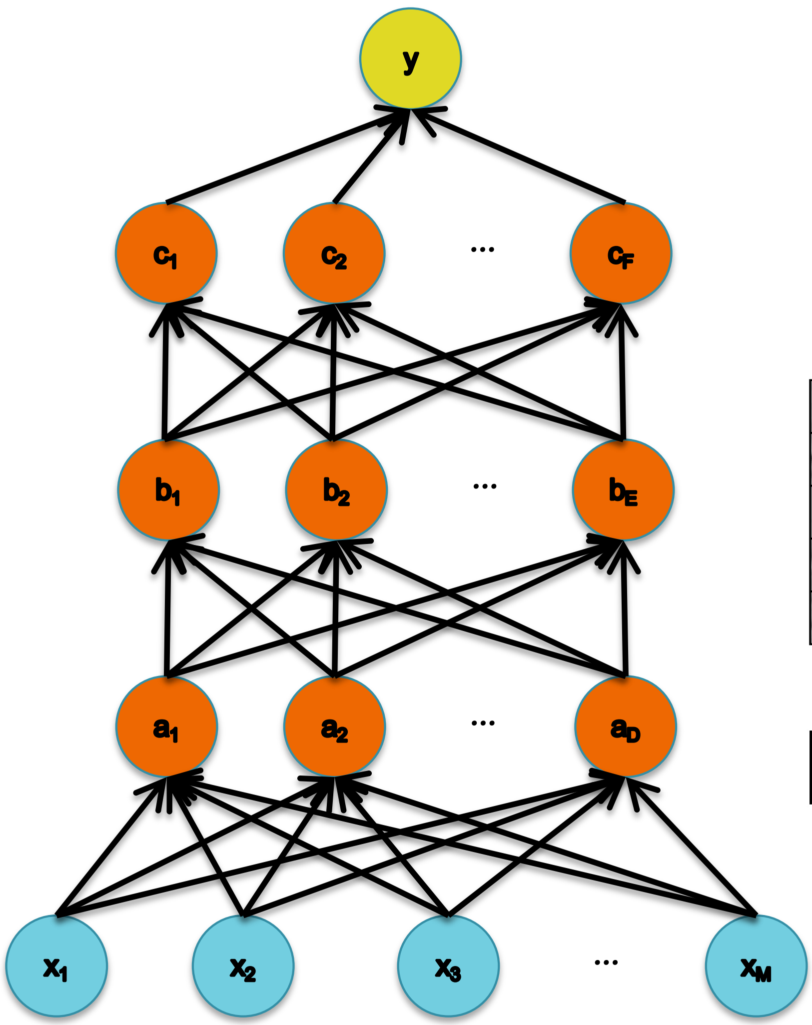
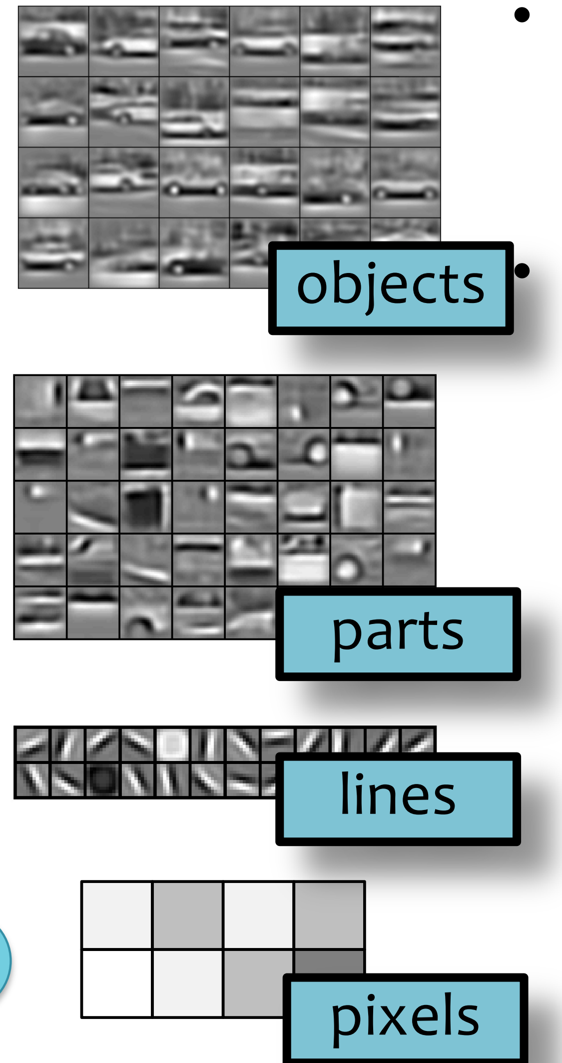
Feature Learning



CBDN on Cars



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