10-601 Introduction to Machine Learning

Machine Learning Department
School of Computer Science
Carnegie Mellon University

Neural Networks

Matt Gormley
Lecture 11
Oct. 8, 2018

Reminders

- Homework 4: Logistic Regression
  - Out: Sun, Sep 30
  - Due: Tue, Oct 9 at 11:59pm
- Homework 5: Neural Networks
  - Out: Tue, Oct 9
  - Due: Sat, Oct 20 at 11:59pm

Q&A

Neural Networks Outline

- **Logistic Regression (Recap)**
  - Data, Model, Learning, Prediction
- **Neural Networks**
  - A Recipe for Machine Learning
  - Visual Notation for Neural Networks
  - Example: Logistic Regression Output Surface
  - 2-Layer Neural Network
  - 3-Layer Neural Network
- **Neural Net Architectures**
  - Objective Functions
  - Activation Functions
- **Backpropagation**
  - Basic Chain Rule (of calculus)
  - Chain Rule for Arbitrary Computation Graph
  - Backpropagation Algorithm
  - Module-based Automatic Differentiation (Autodiff)

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

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

   - Loss function

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

Examples: Linear regression, Logistic regression, Neural Network

Examples: Mean-squared error, Cross Entropy

Background

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2. Choose each of these:

– Decision function

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– 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

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

$\boldsymbol{y}_i)$

2. Choose each of t

– Decision functio

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

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opposite 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

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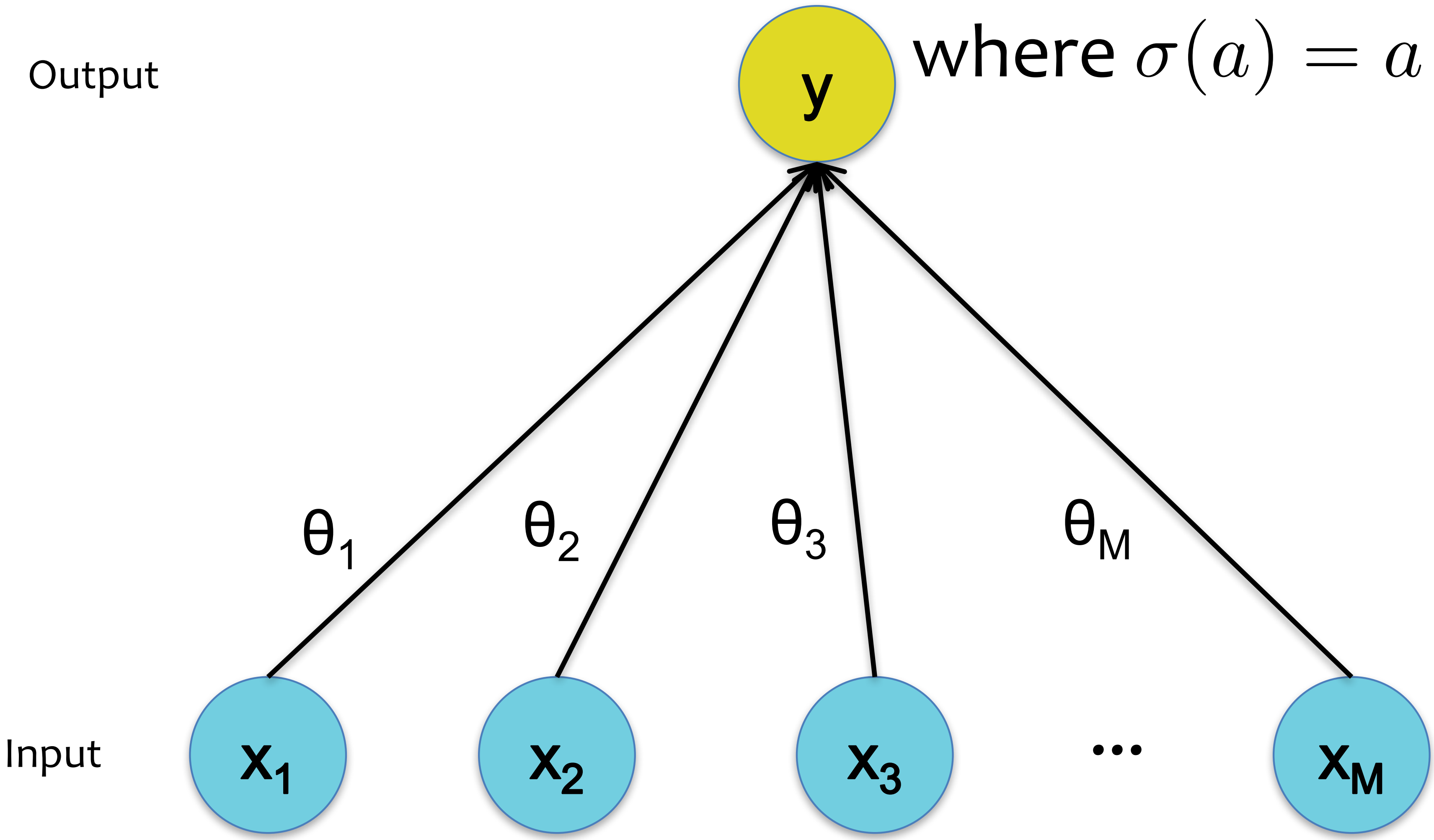
Decision Functions

Linear Regression

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

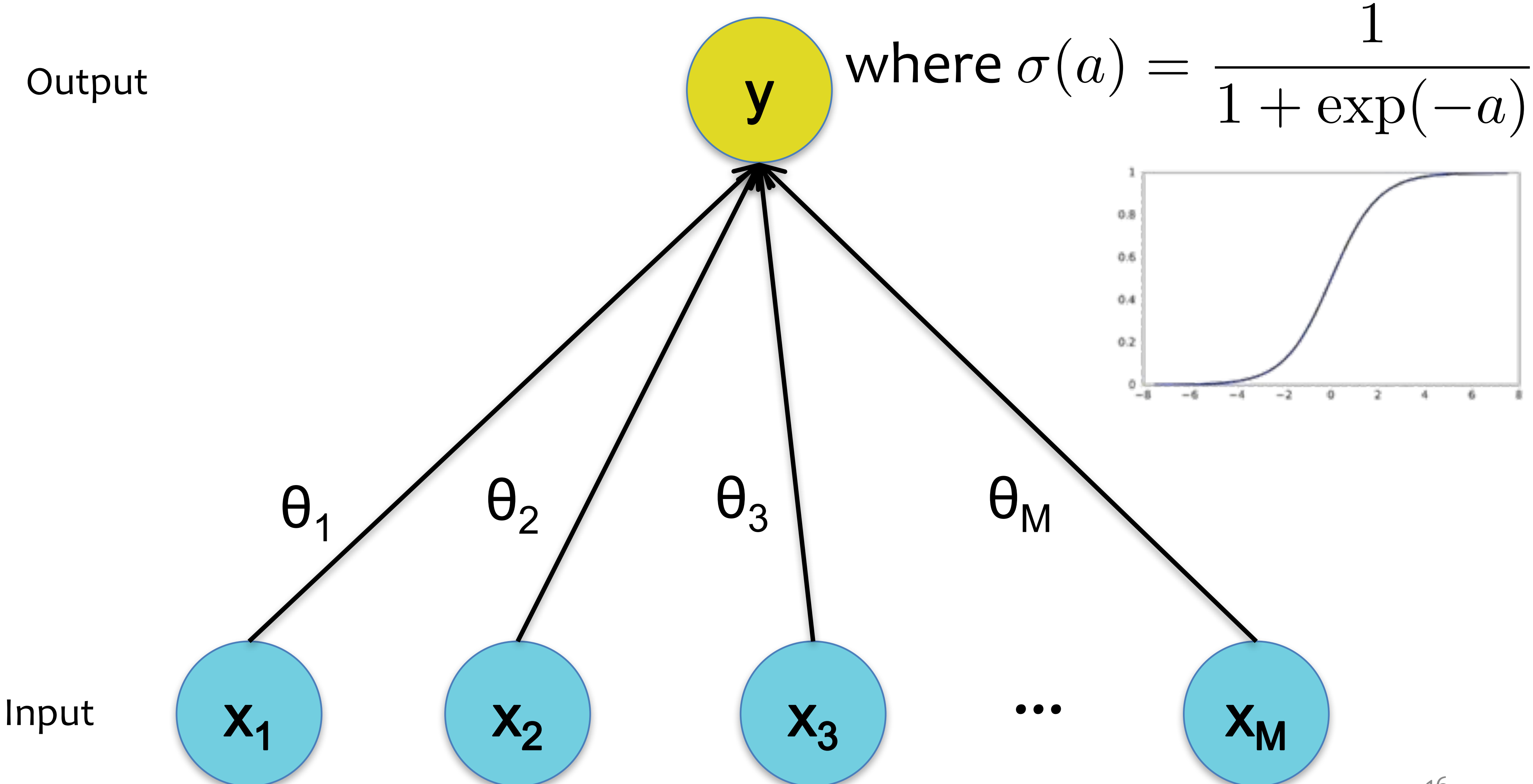
where $\sigma(a) = a$



Logistic Regression

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

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



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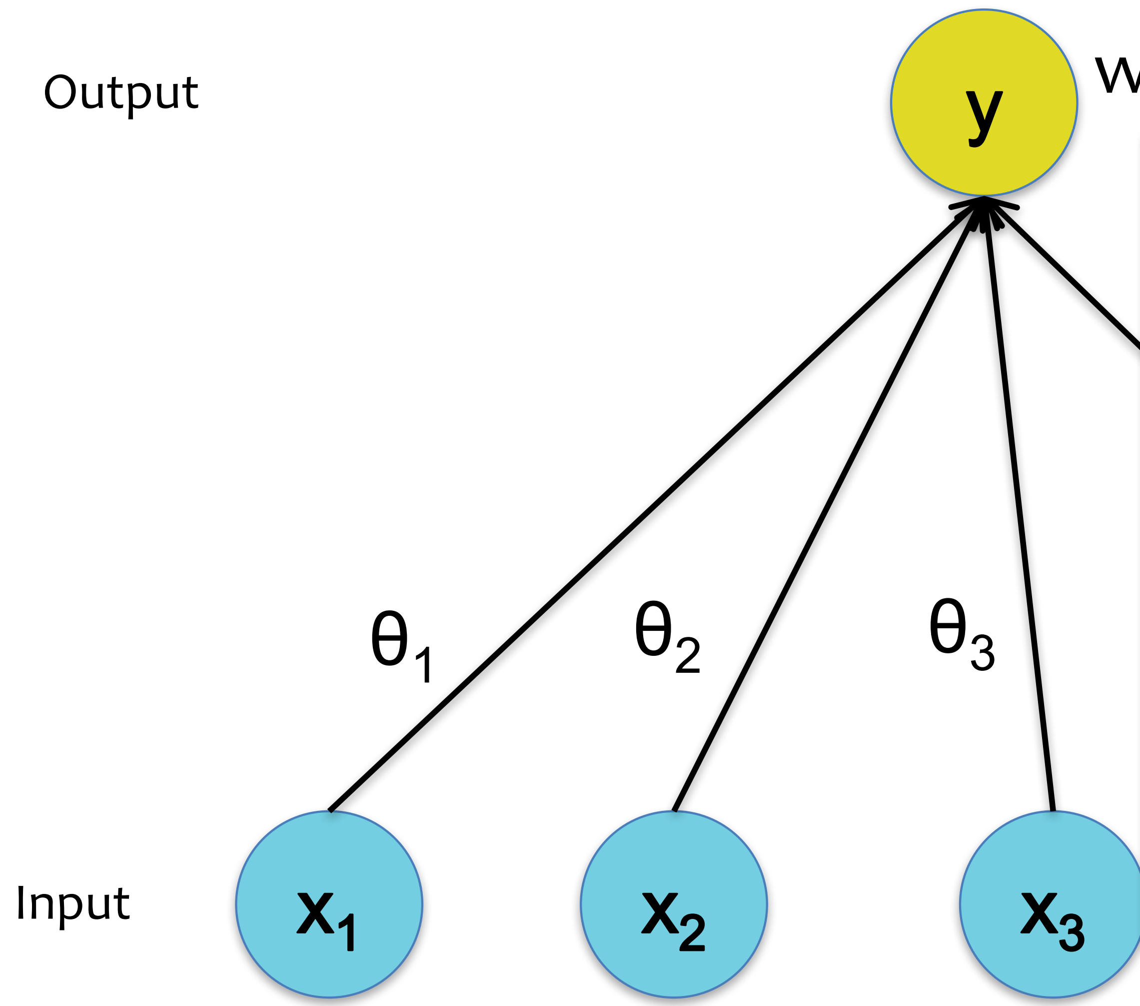

Face *Face* *Not a face*

Decision Functions

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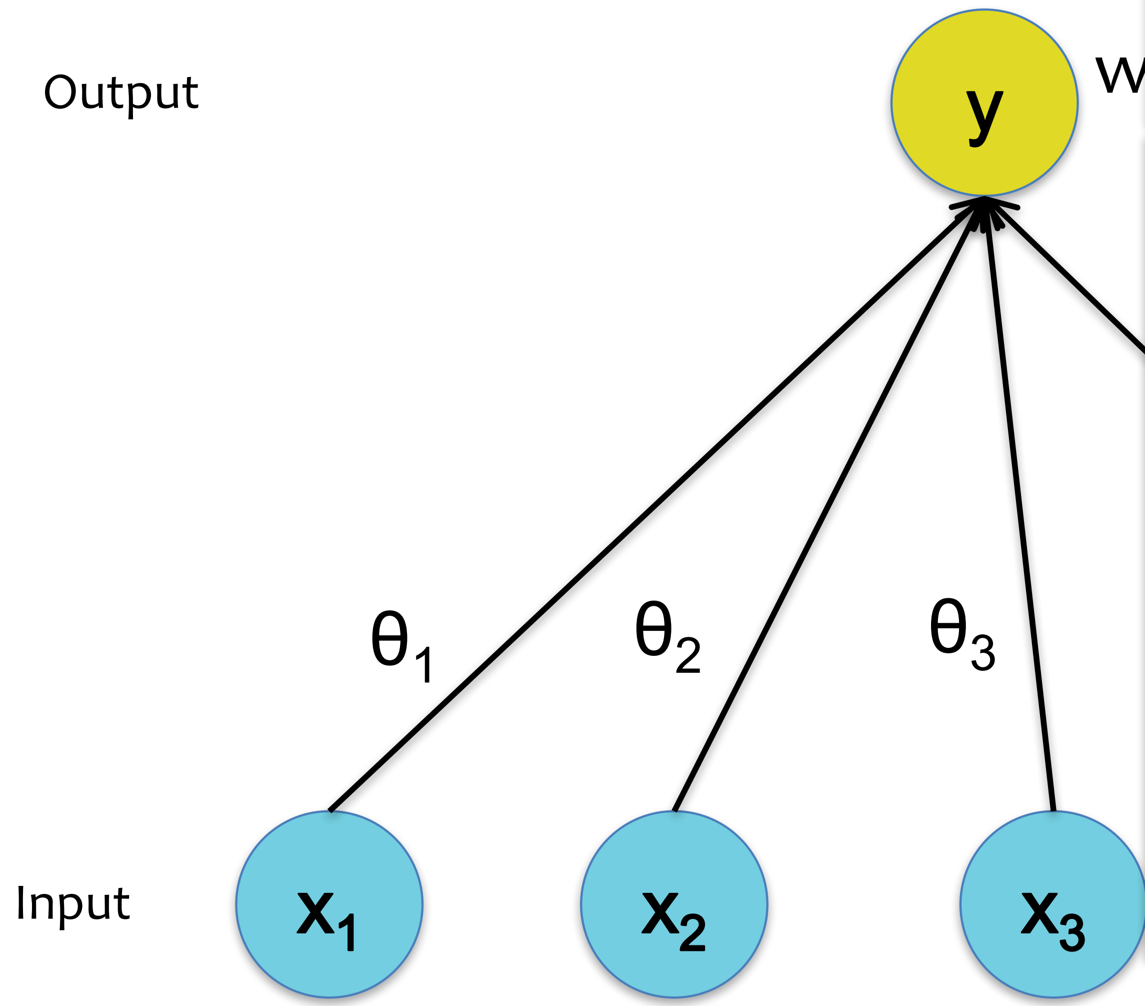
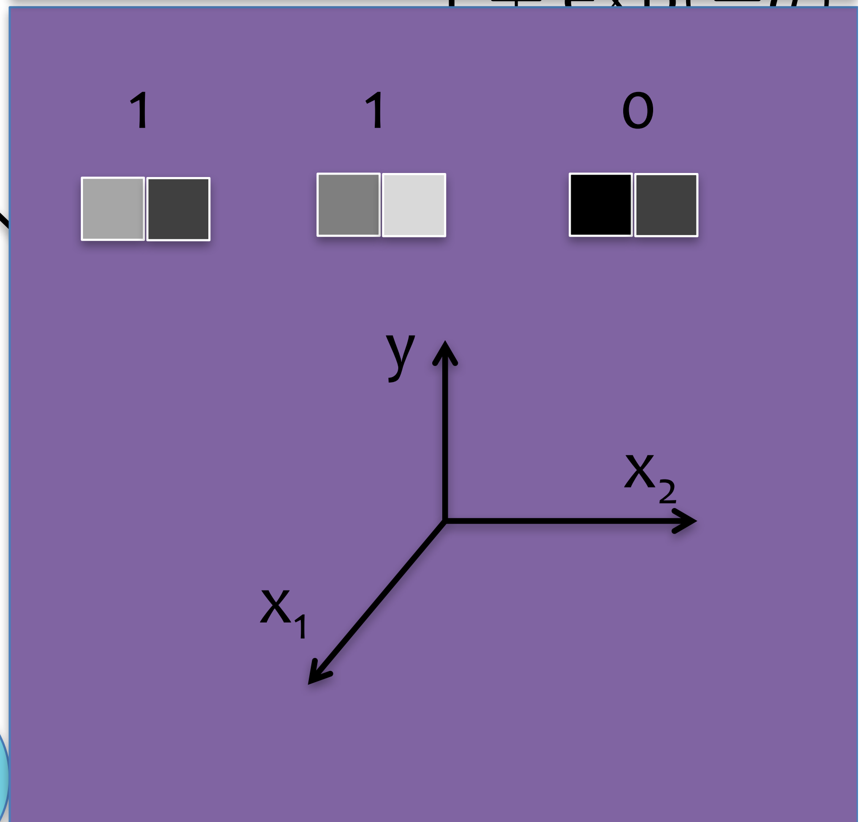


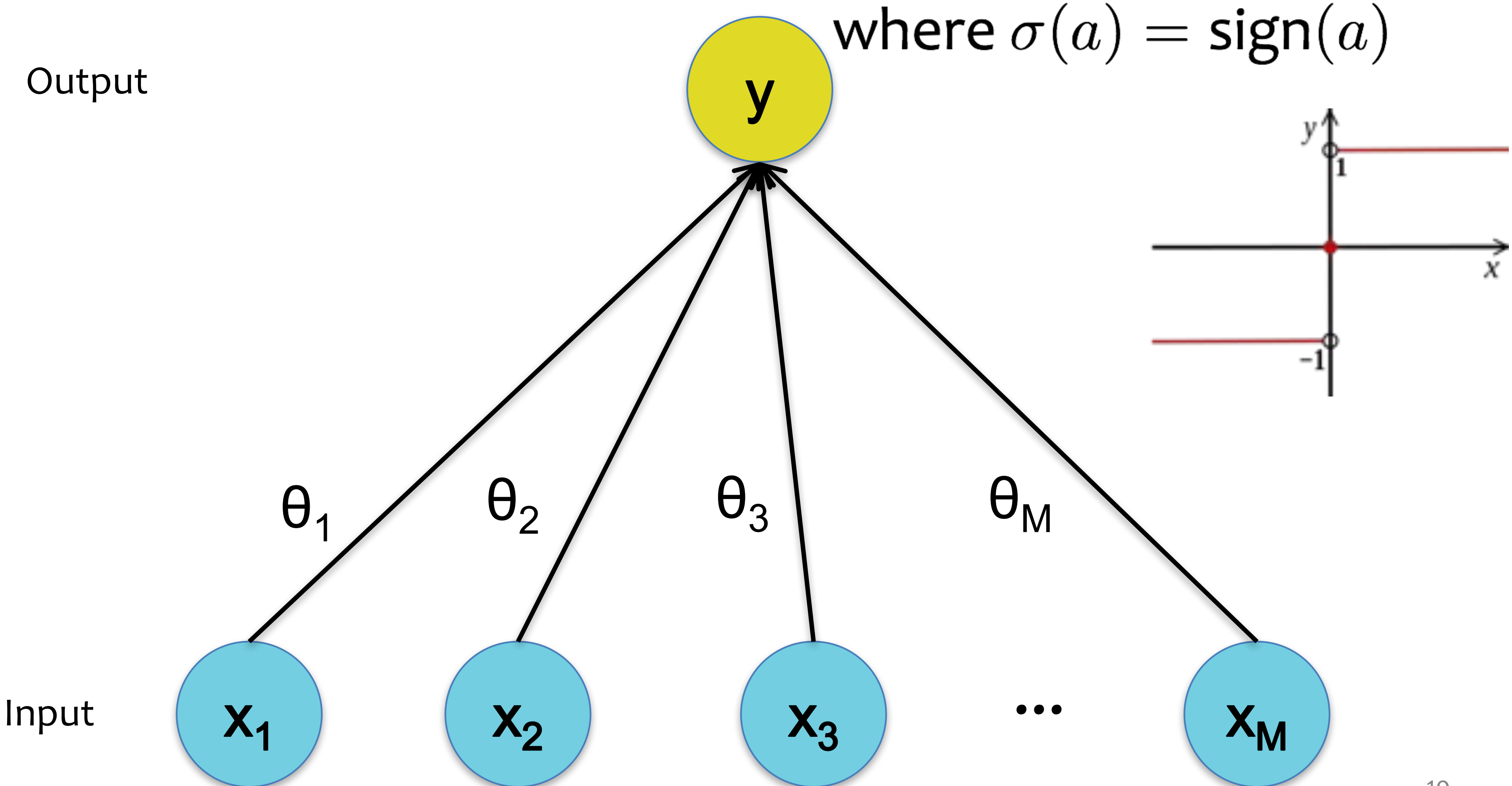
In-Class Example



Perceptron

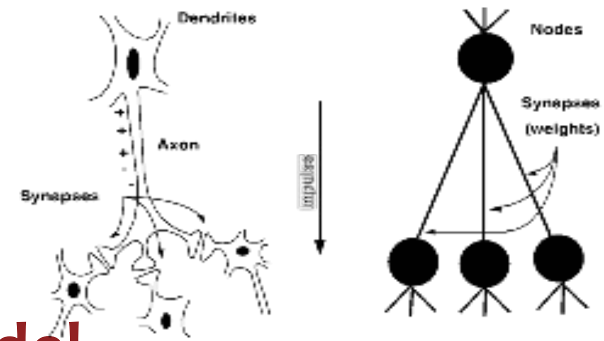
$$y = h_{\boldsymbol{\theta}}(\boldsymbol{x}) = \sigma(\boldsymbol{\theta}^T \boldsymbol{x})$$

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



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

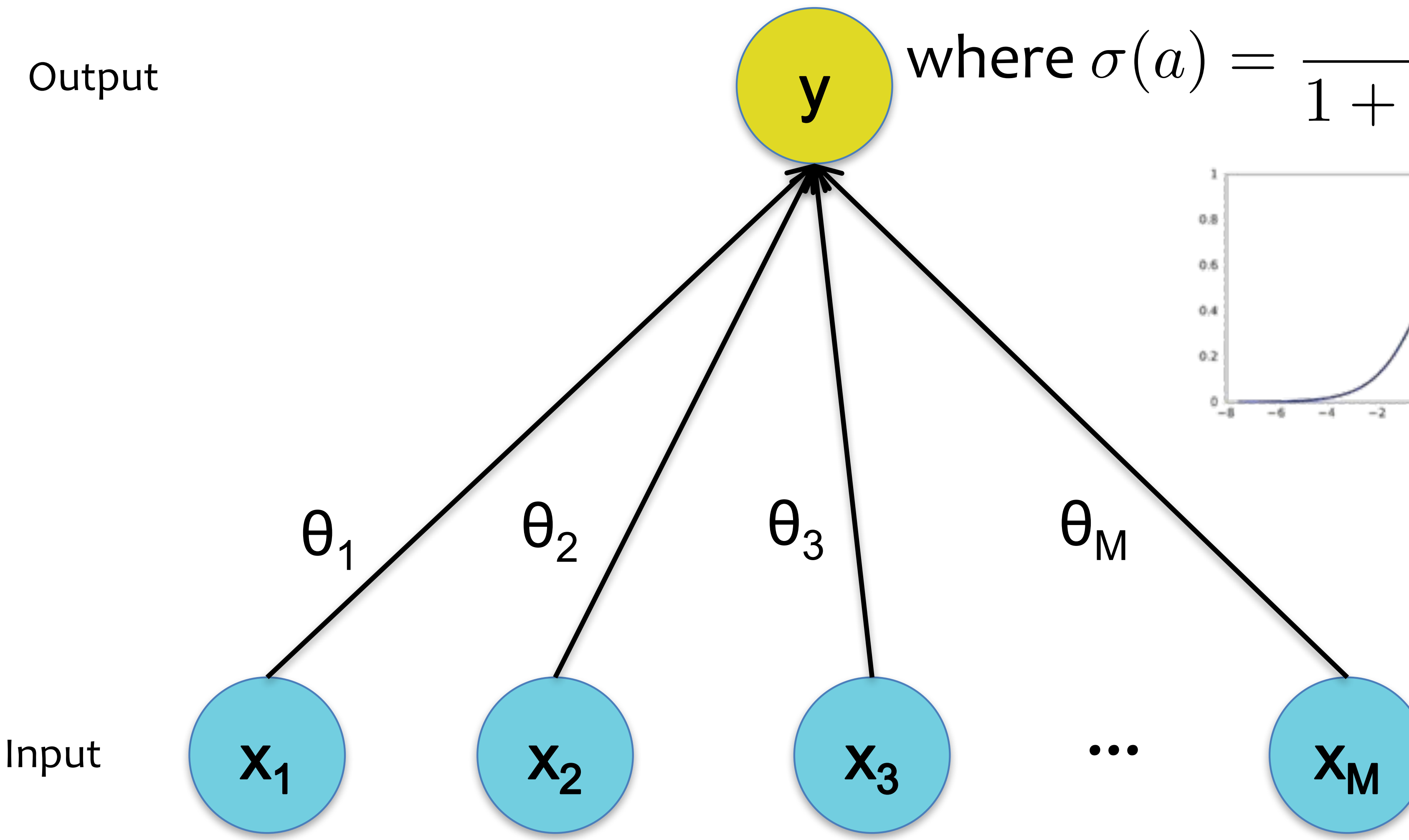
- Many neuron-like threshold switching units
- Many weighted interconnections among units
- Highly parallel, distributed processes

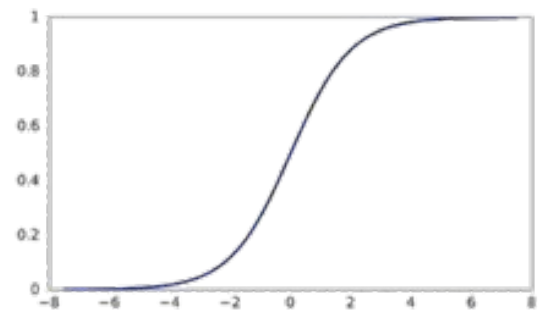
Slide adapted from Eric Xing

Logistic Regression

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

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





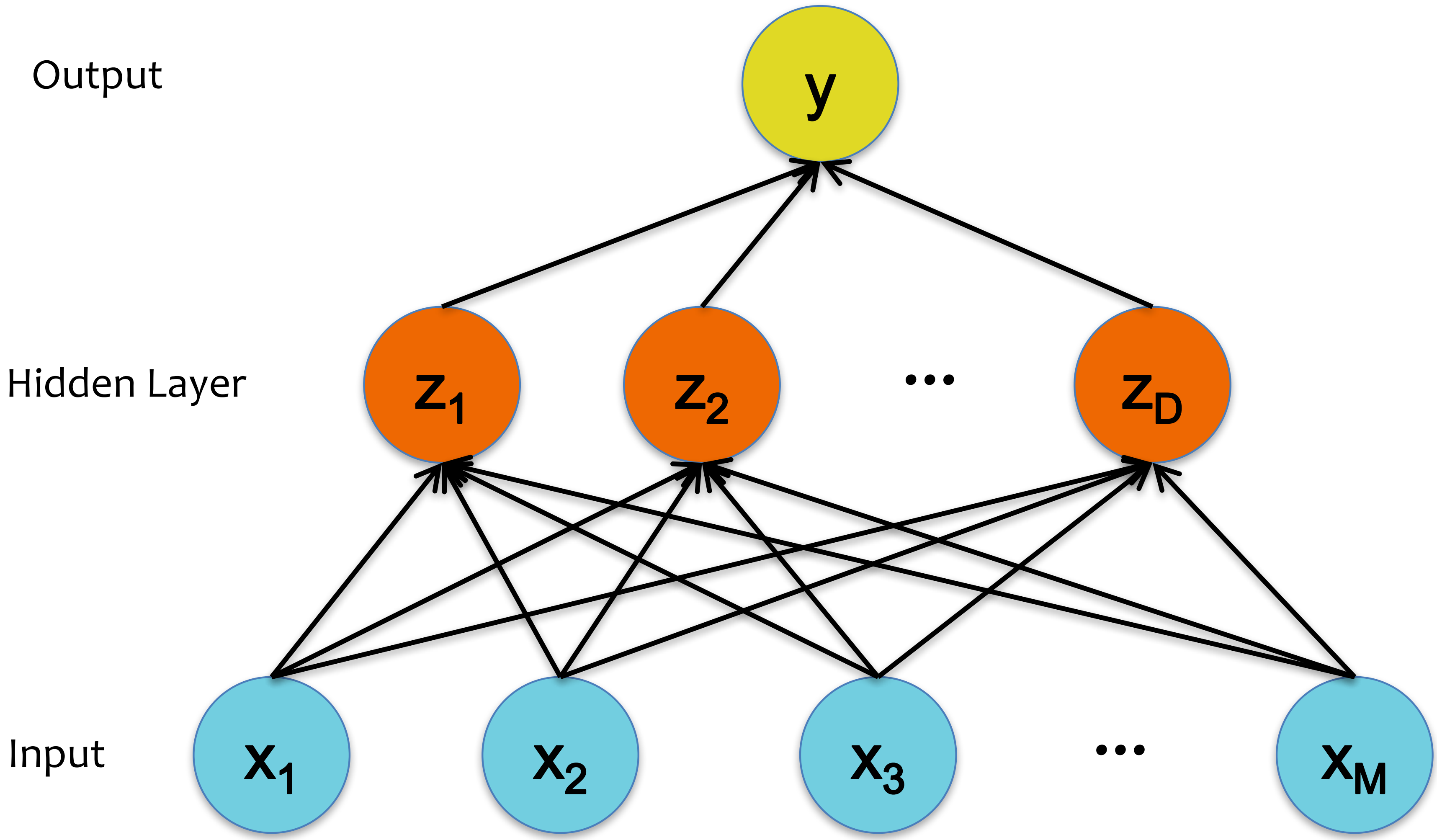
Neural Networks

Chalkboard

- Example: Neural Network w/1 Hidden Layer
- Example: Neural Network w/2 Hidden Layers
- Example: Feed Forward Neural Network

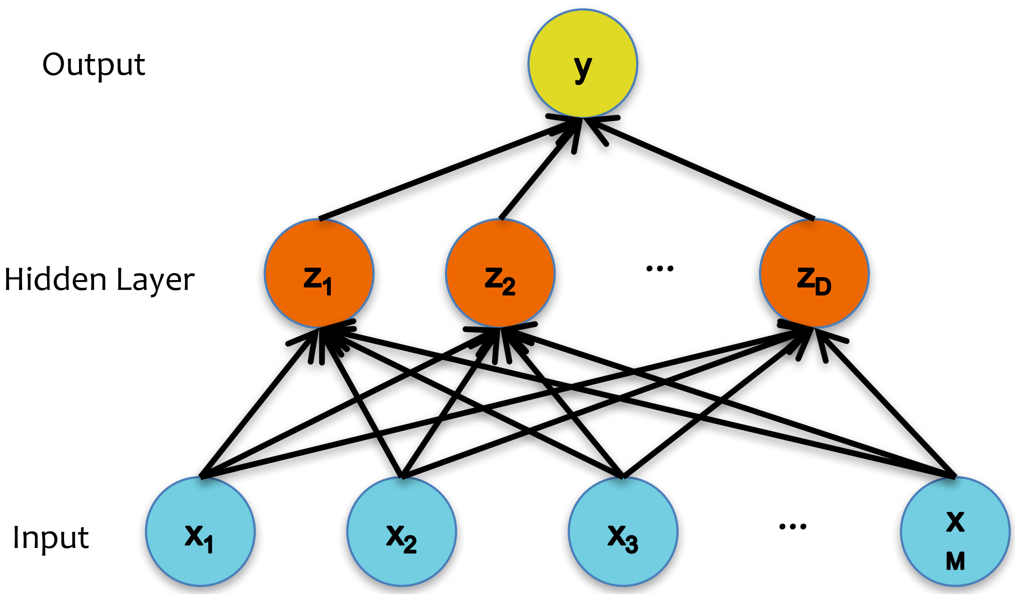
Decision Functions

Neural Network



Decision Functions

Neural Network



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

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

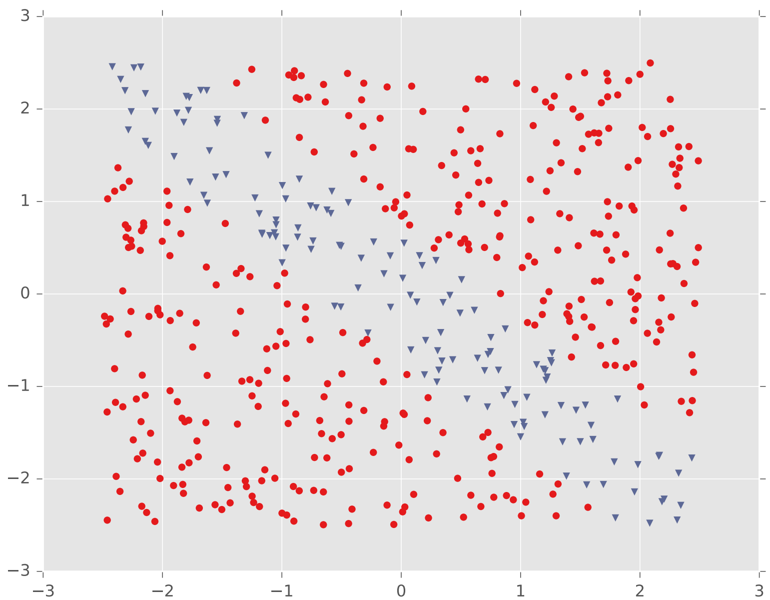
(C) Hidden (sigmoid)
$z_j = \frac{1}{1+\exp(-a_j)}, \quad \forall j$

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

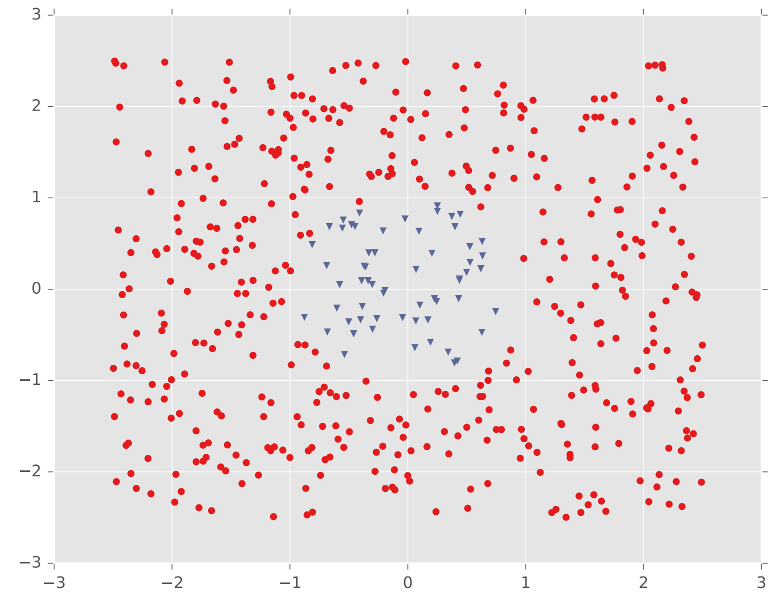
(A) Input
Given $x_i, \quad \forall i$

DECISION BOUNDARY EXAMPLES

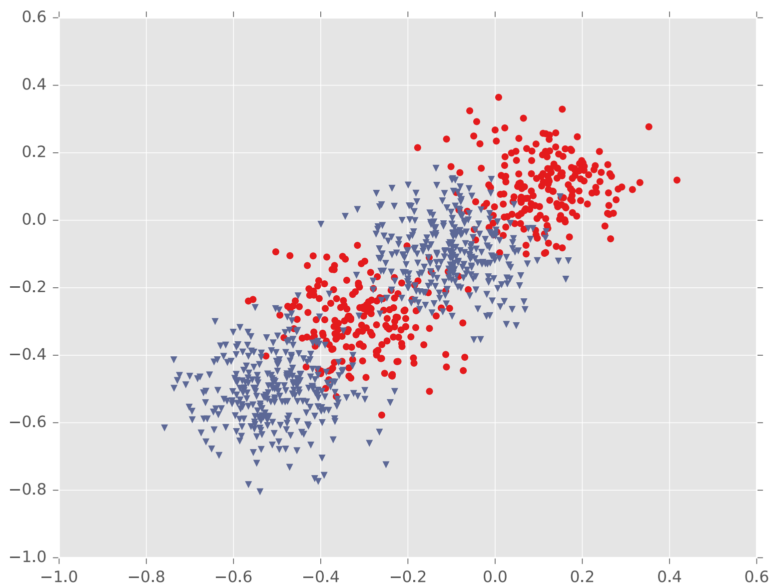
Example #1: Diagonal Band



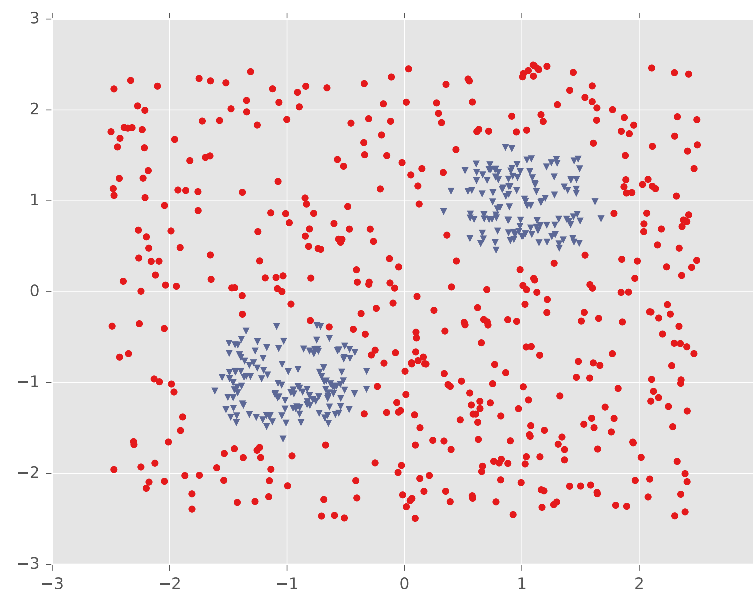
Example #2: One Pocket



Example #3: Four Gaussians



Example #4: Two Pockets



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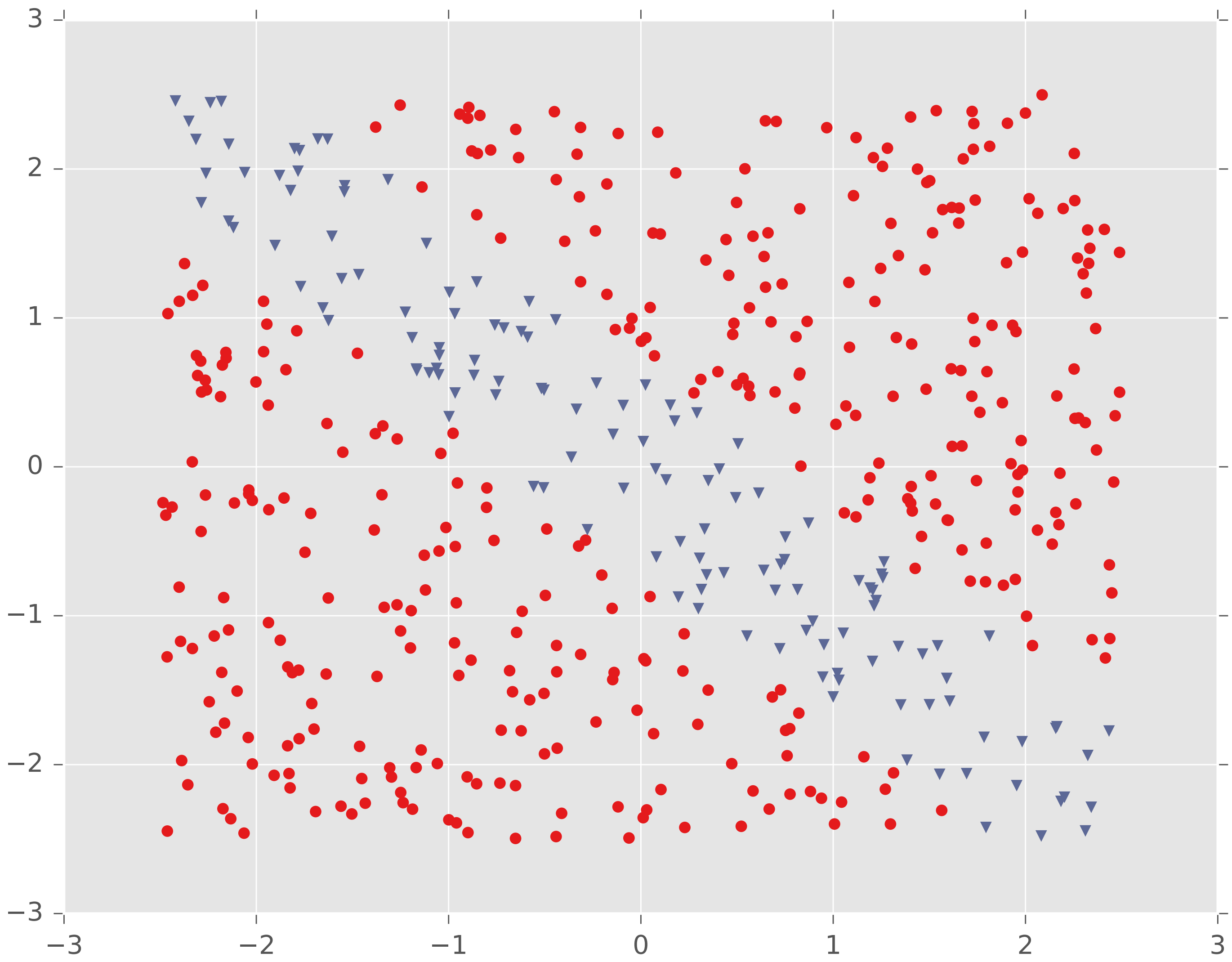

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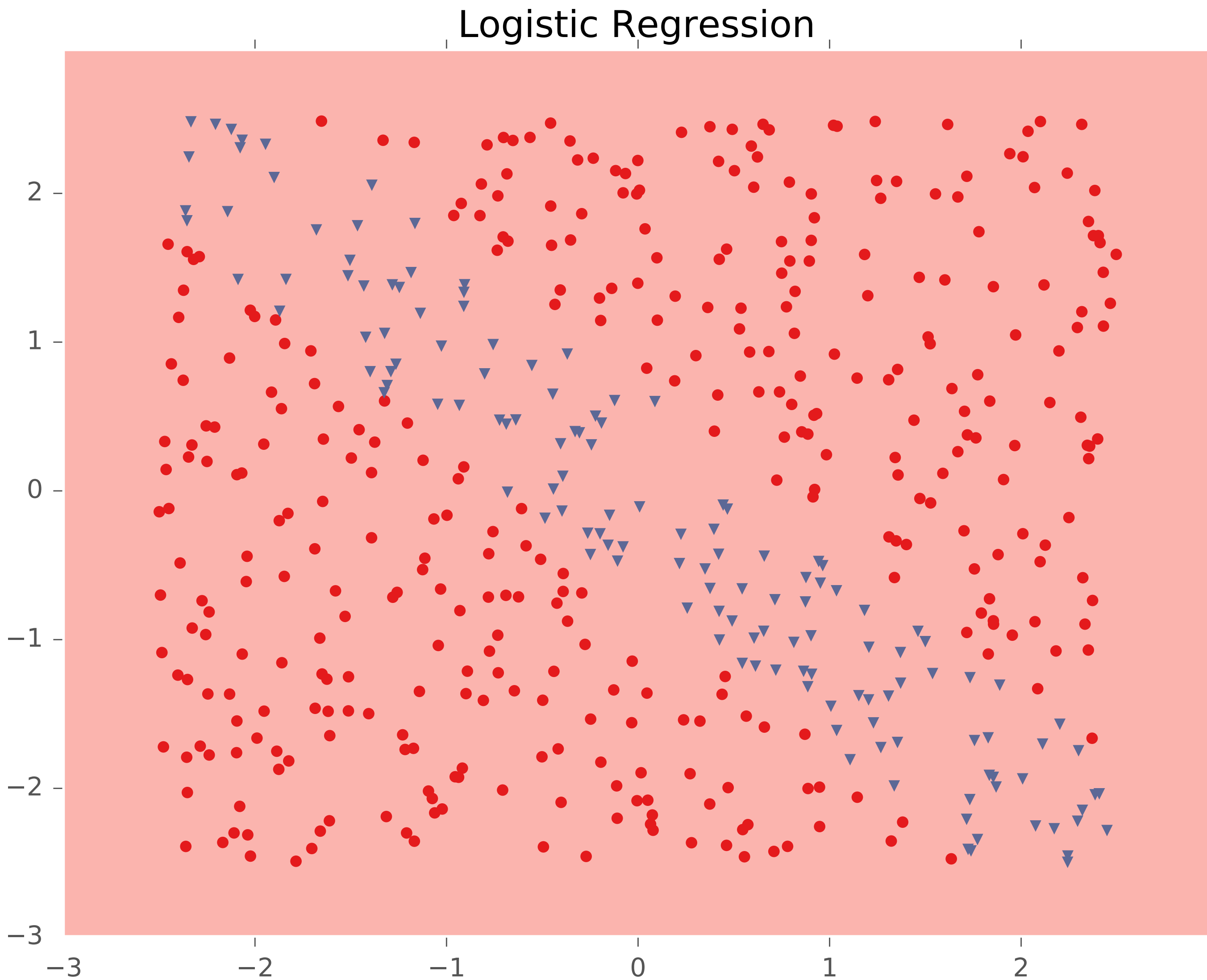

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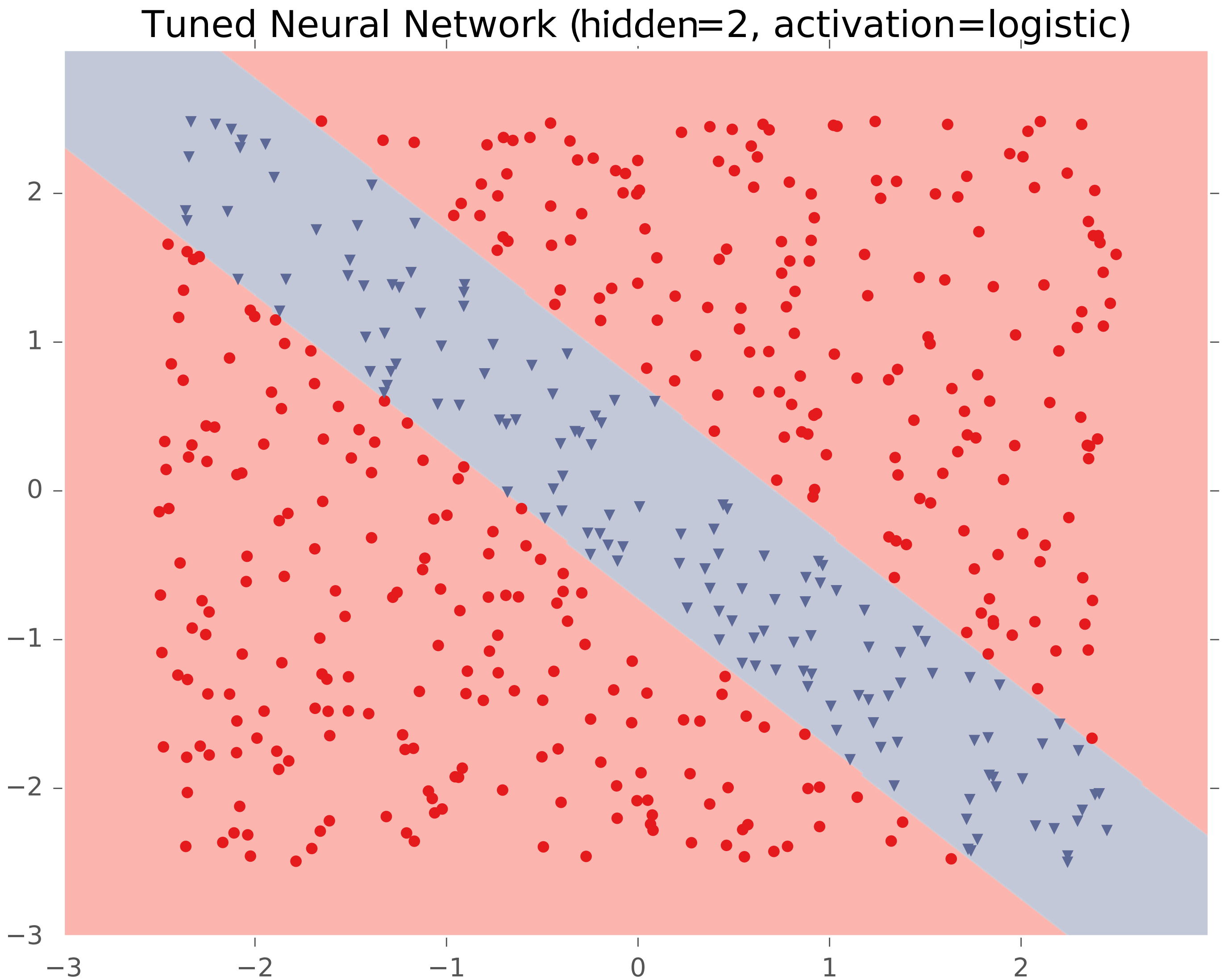

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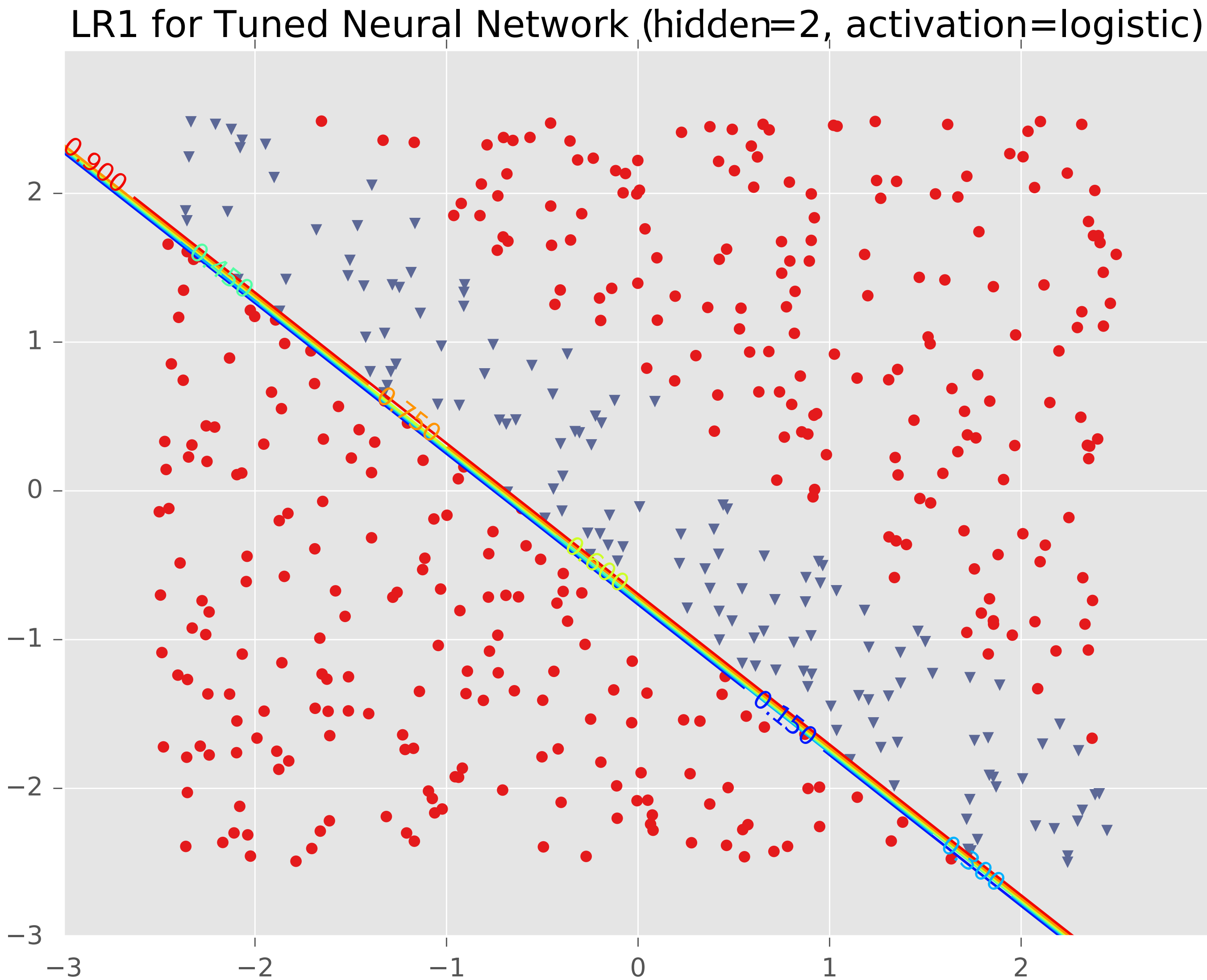

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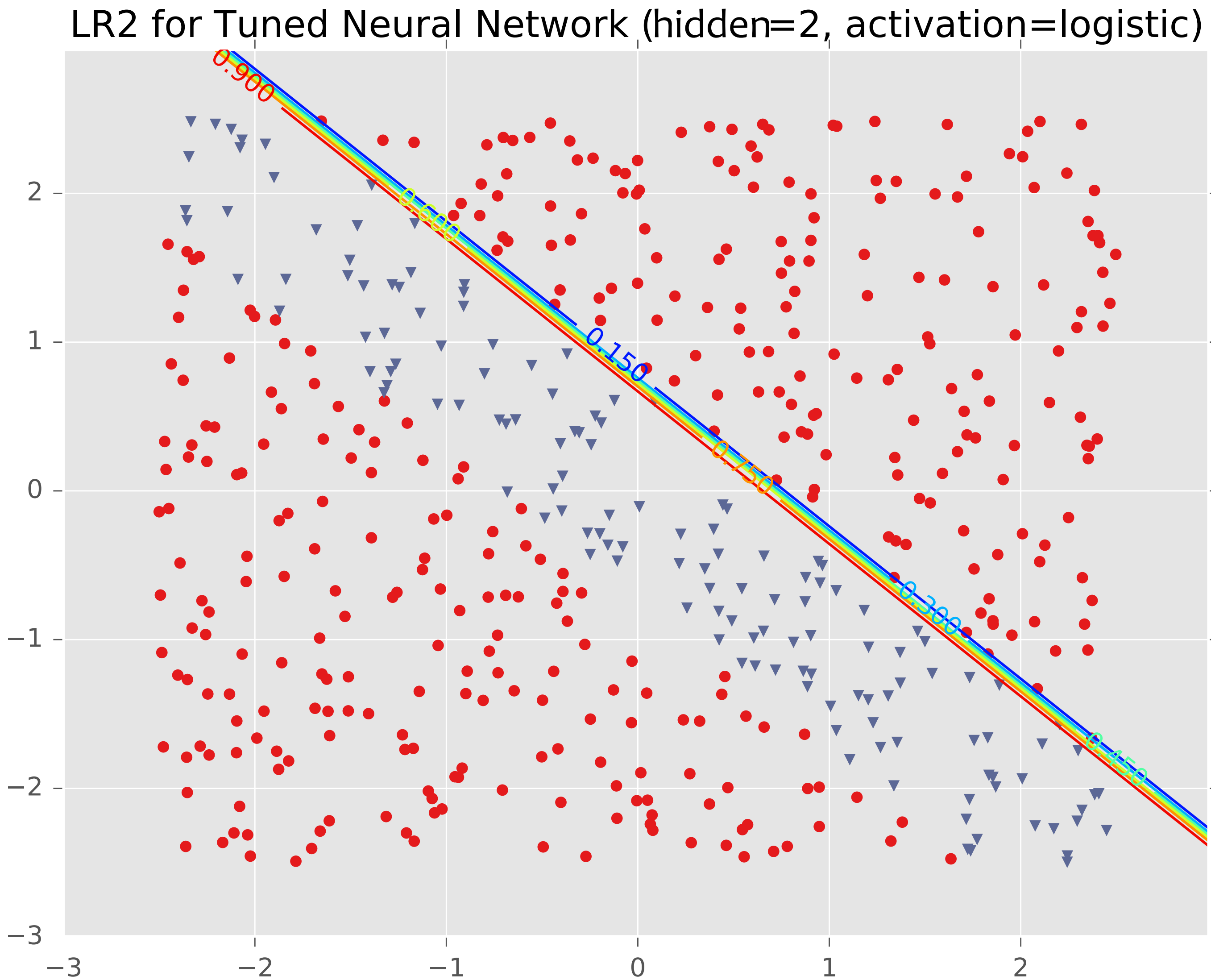

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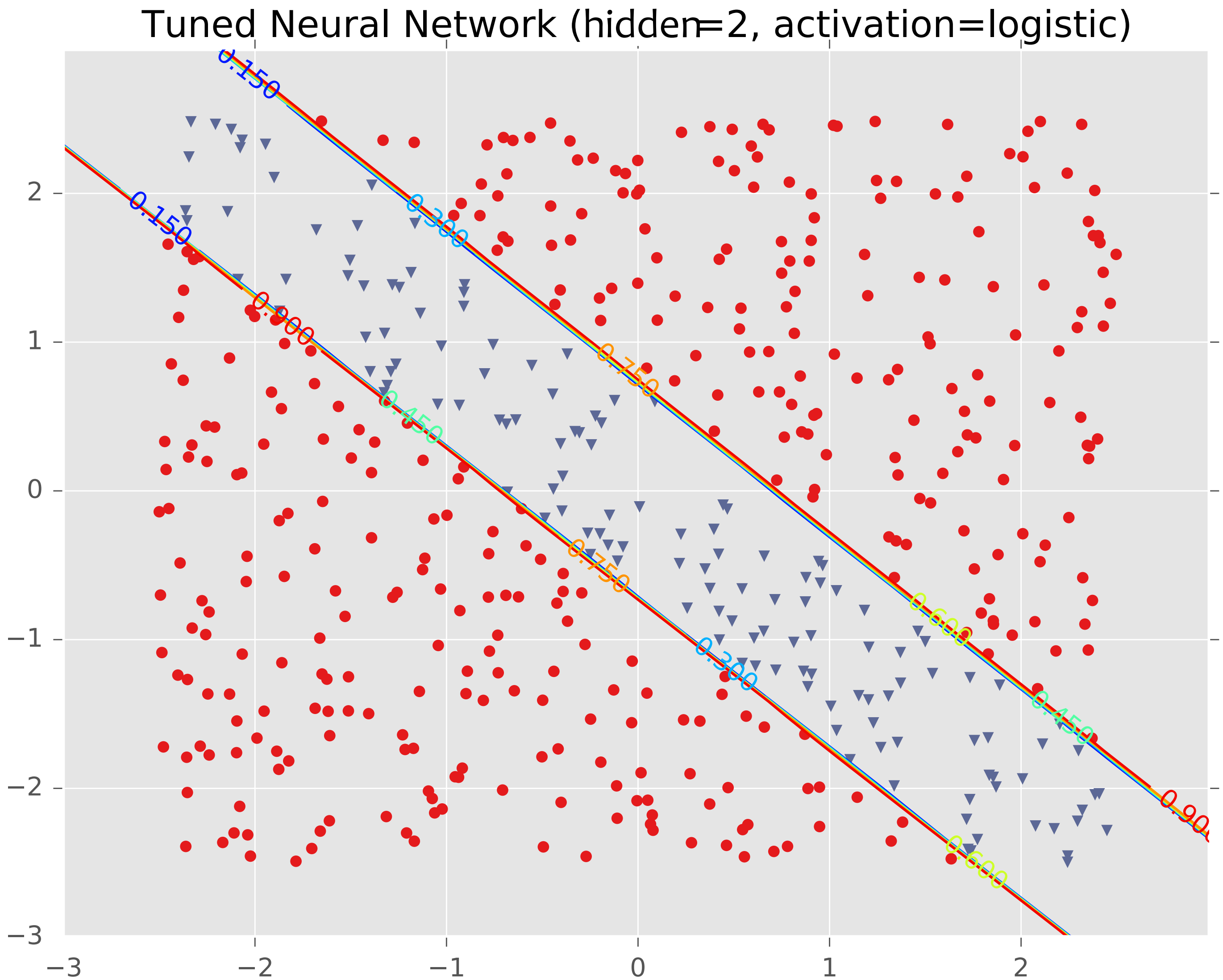

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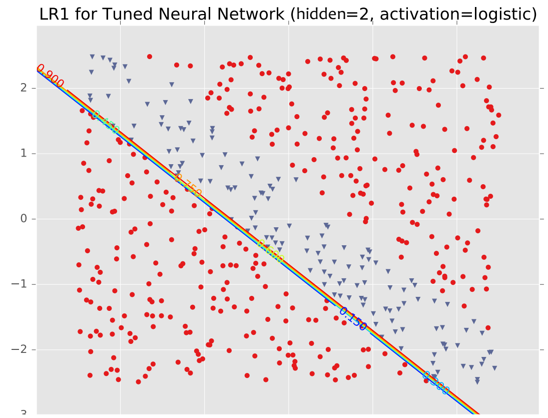

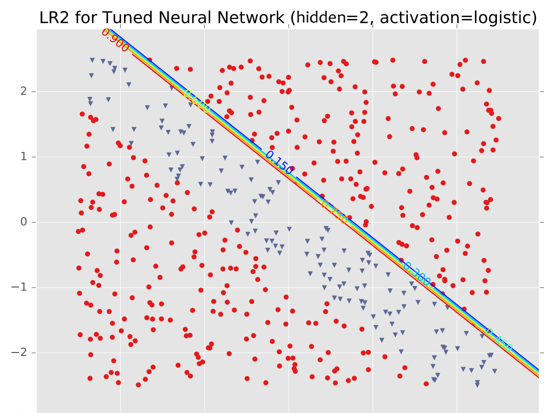

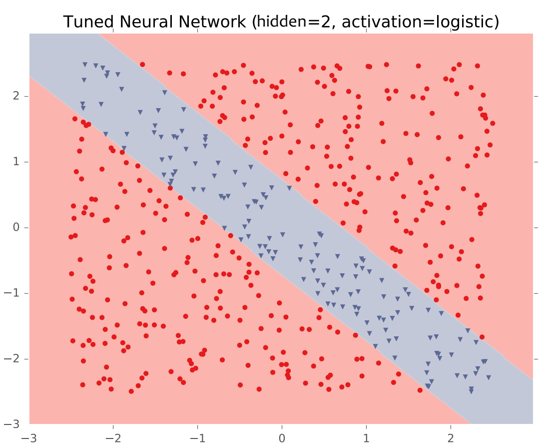

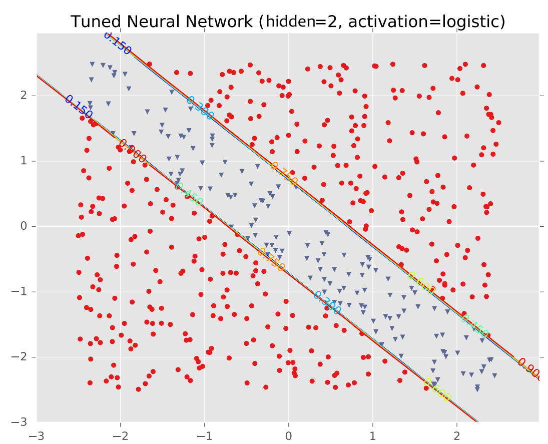

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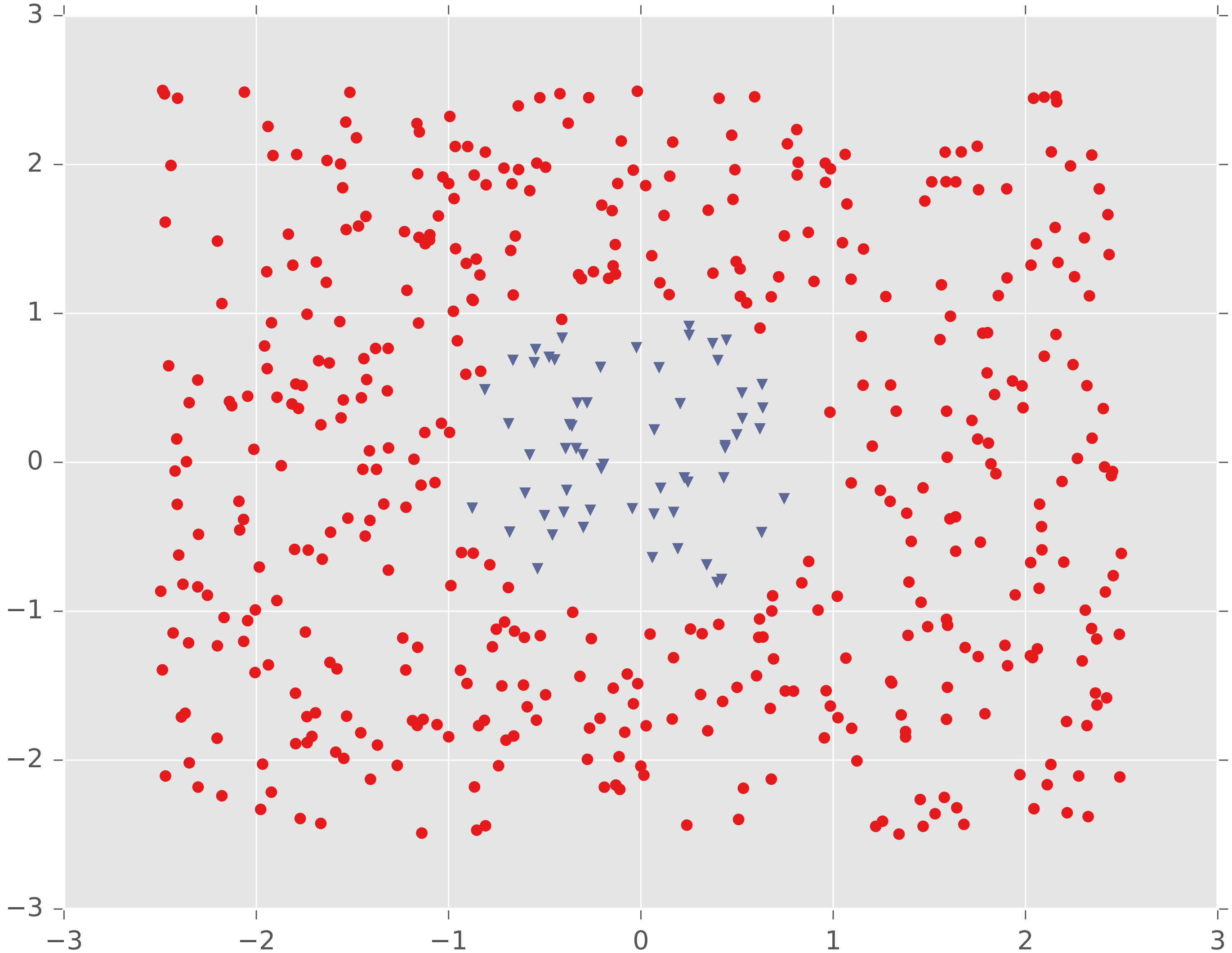

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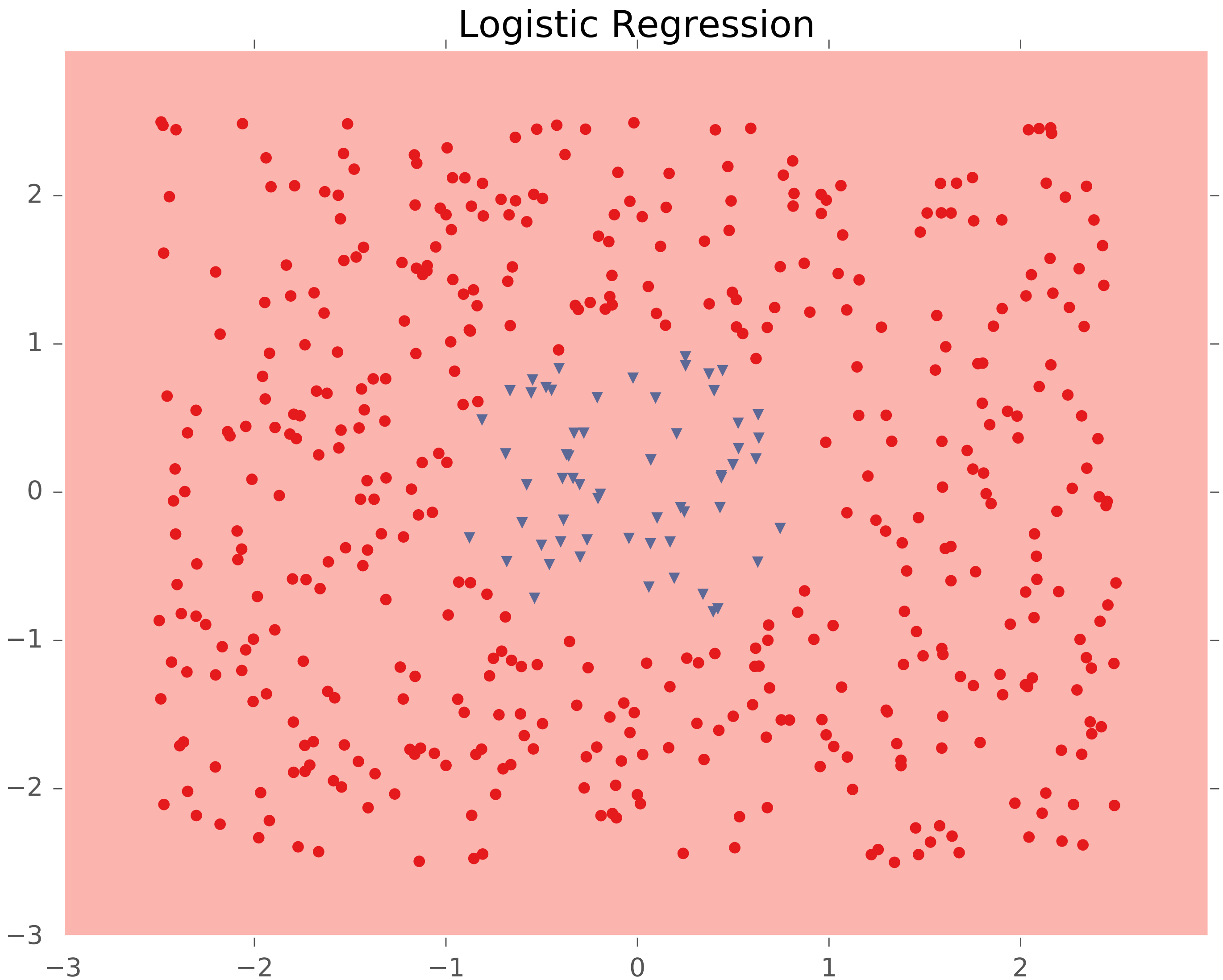

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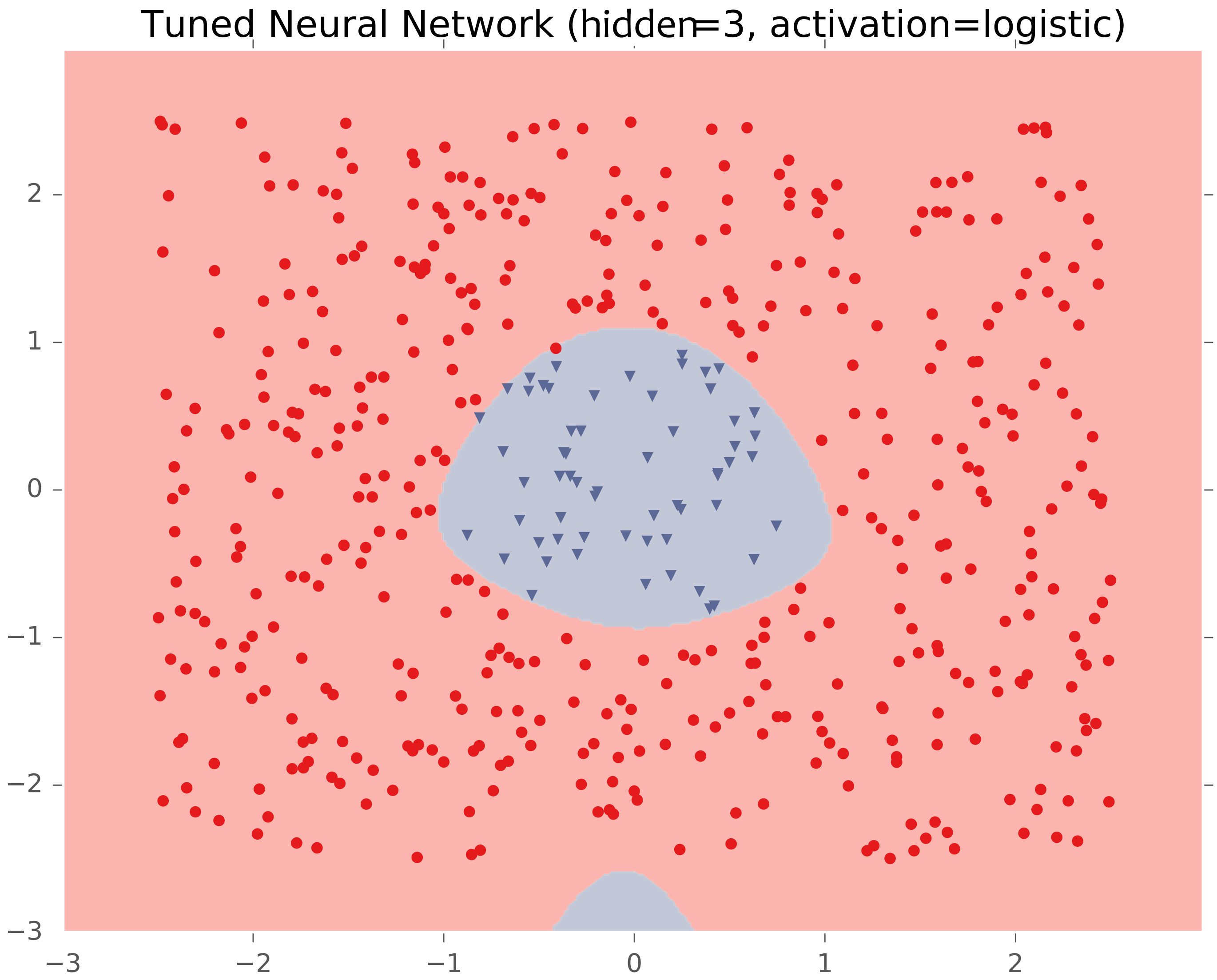

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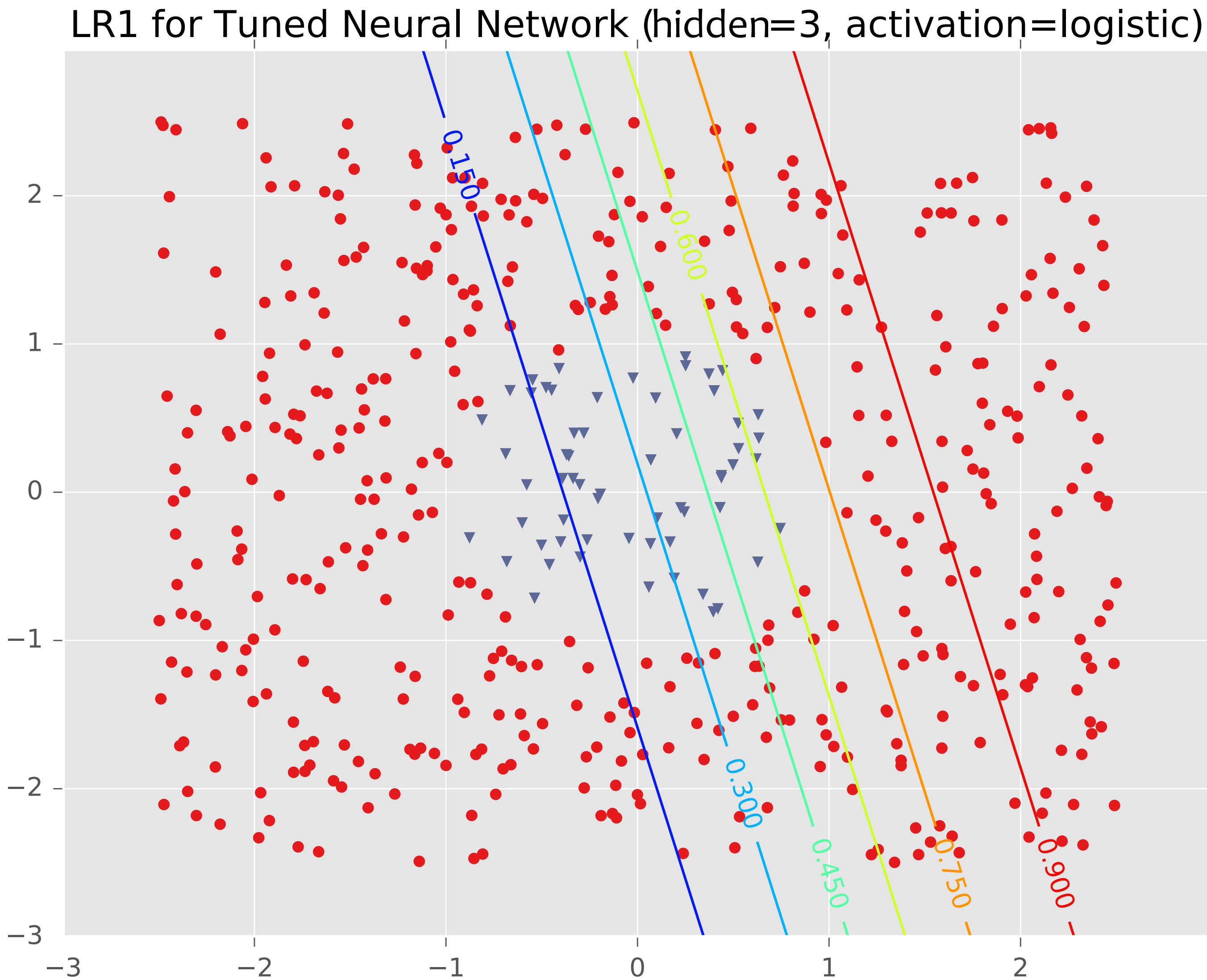

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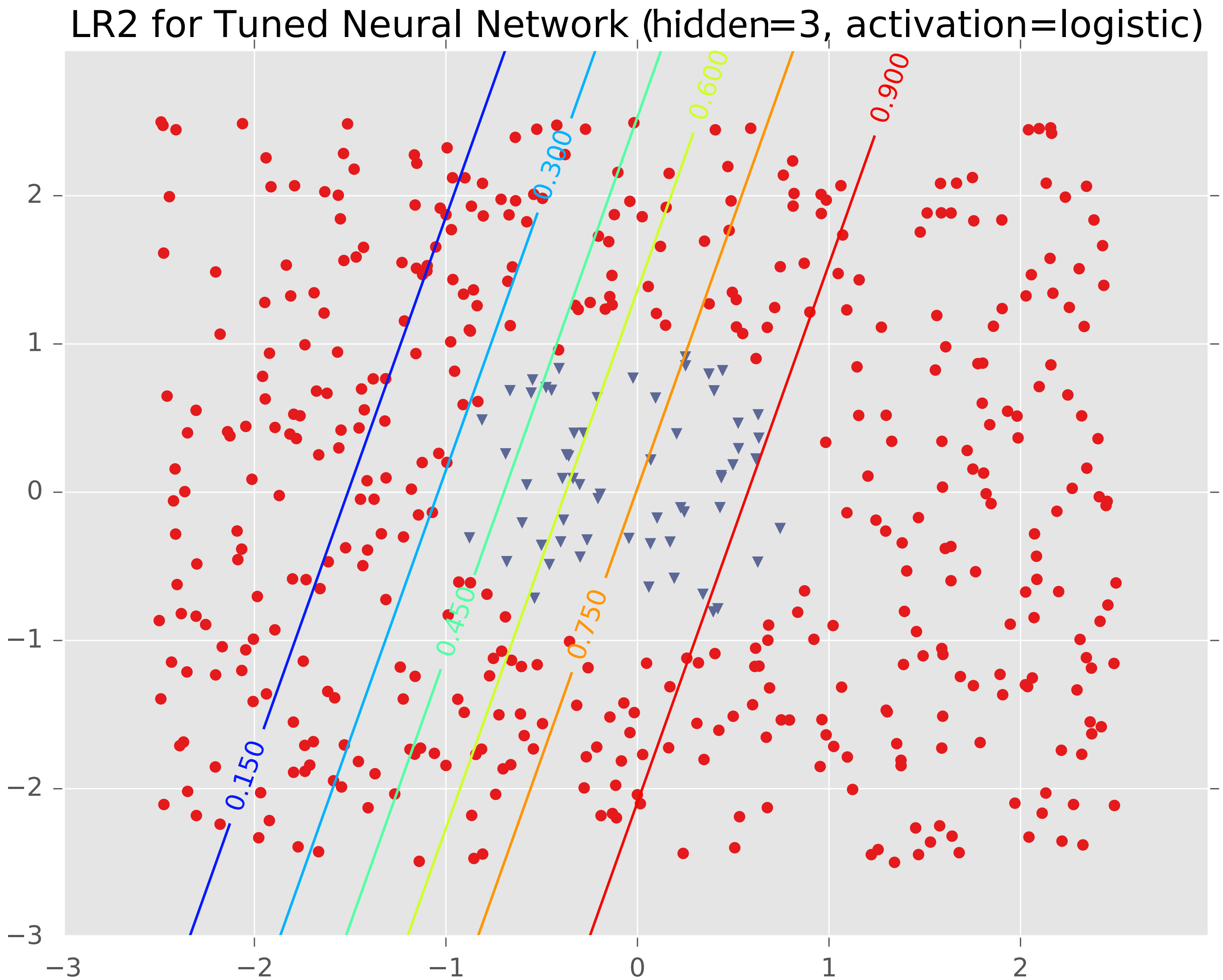

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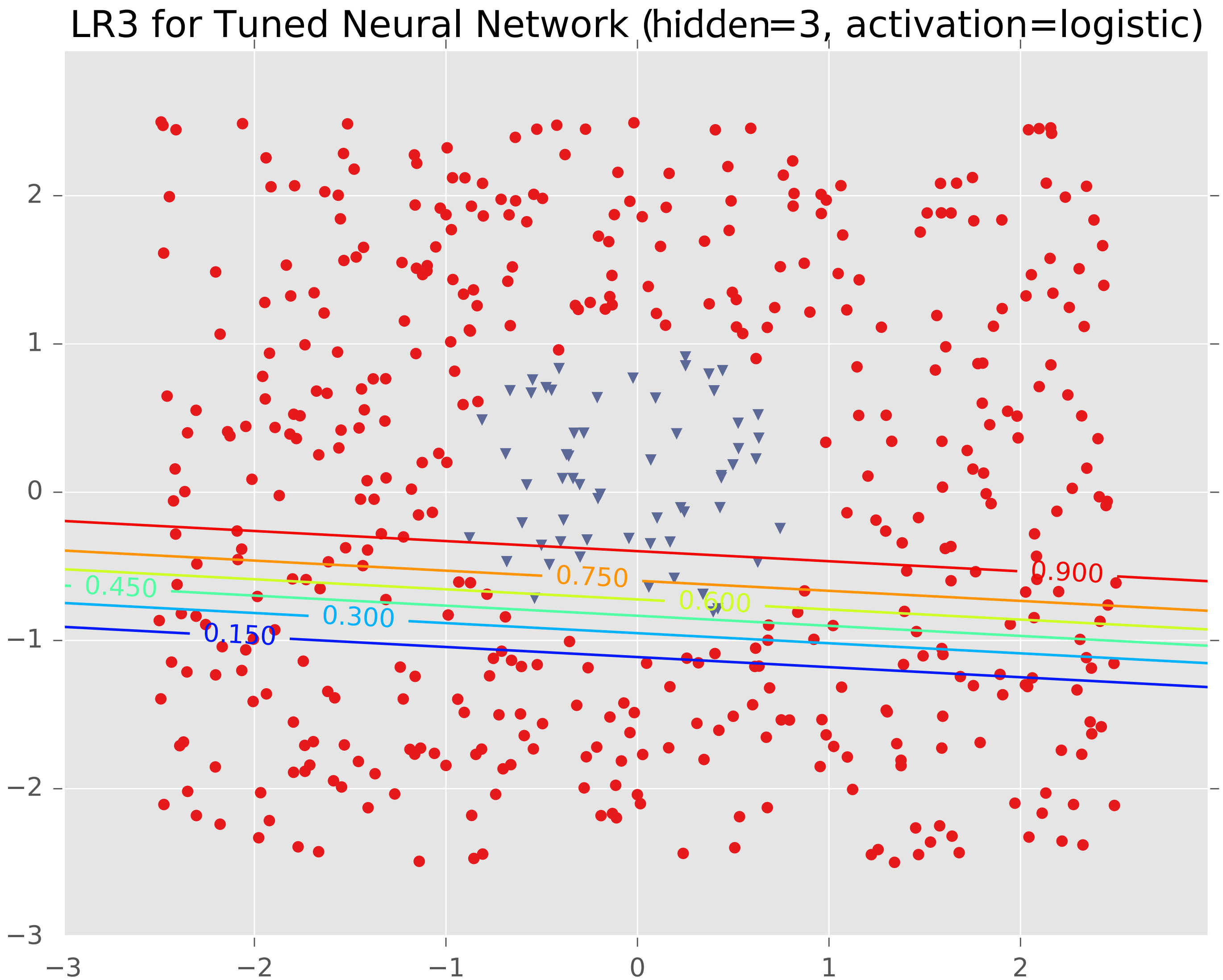

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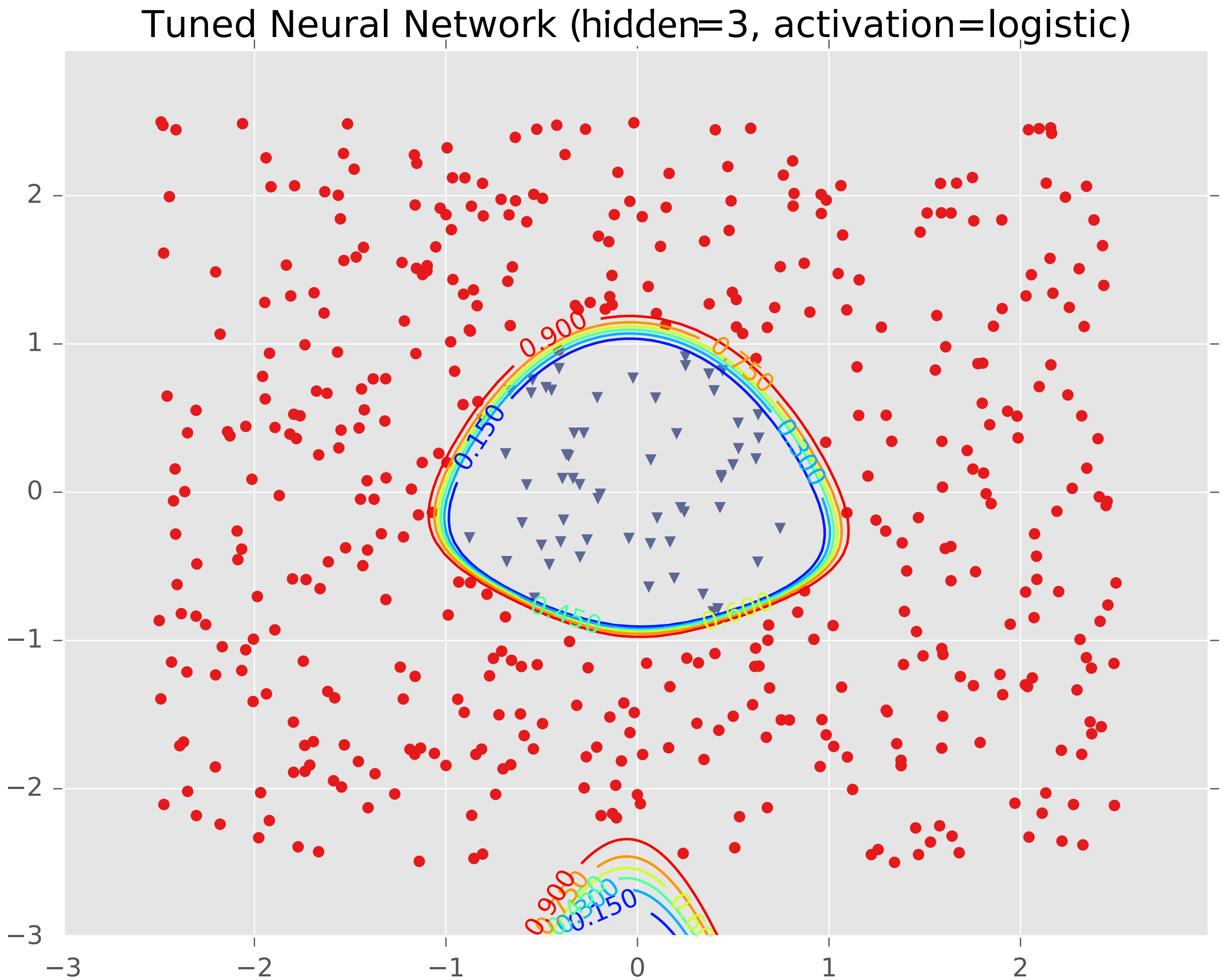

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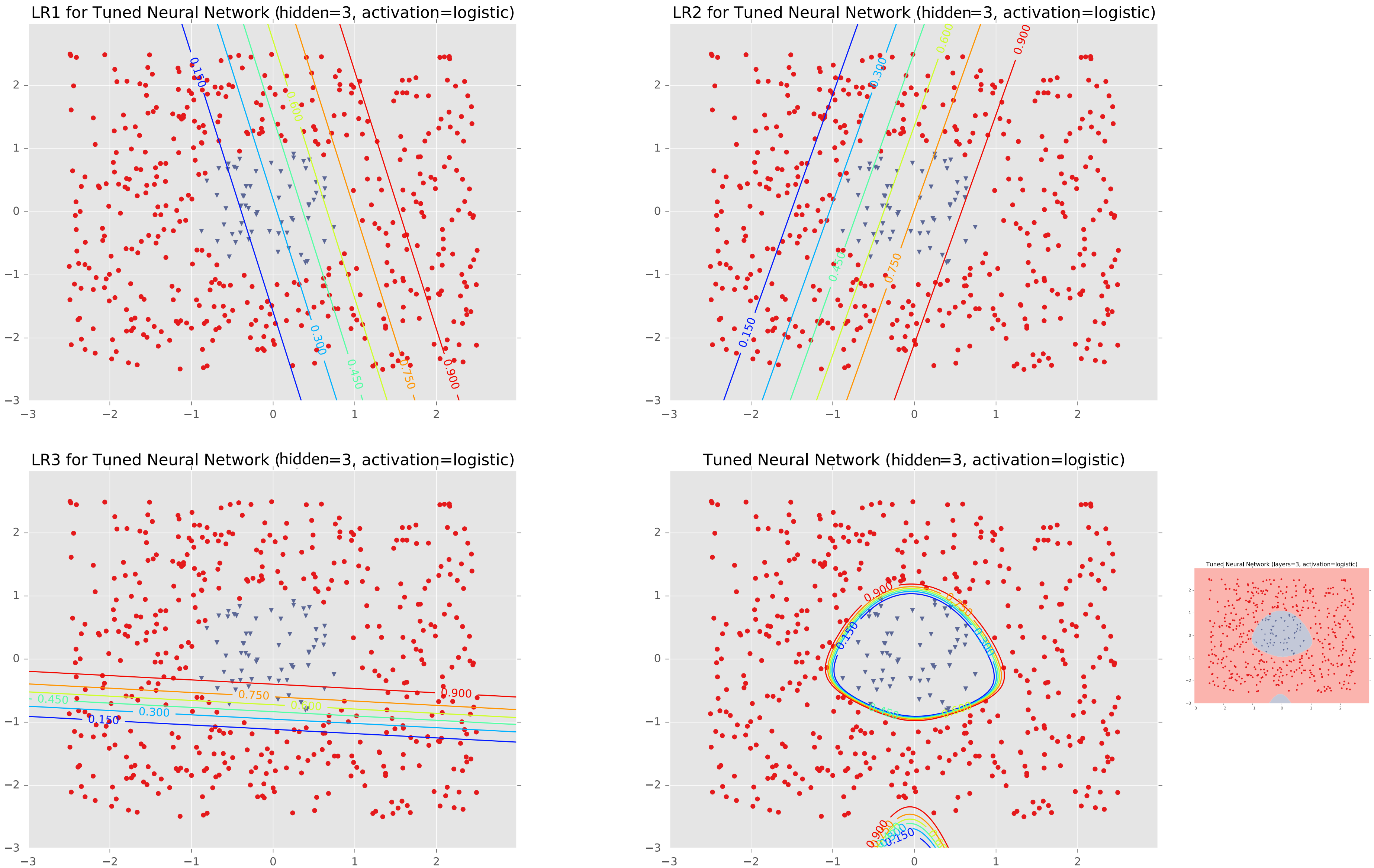

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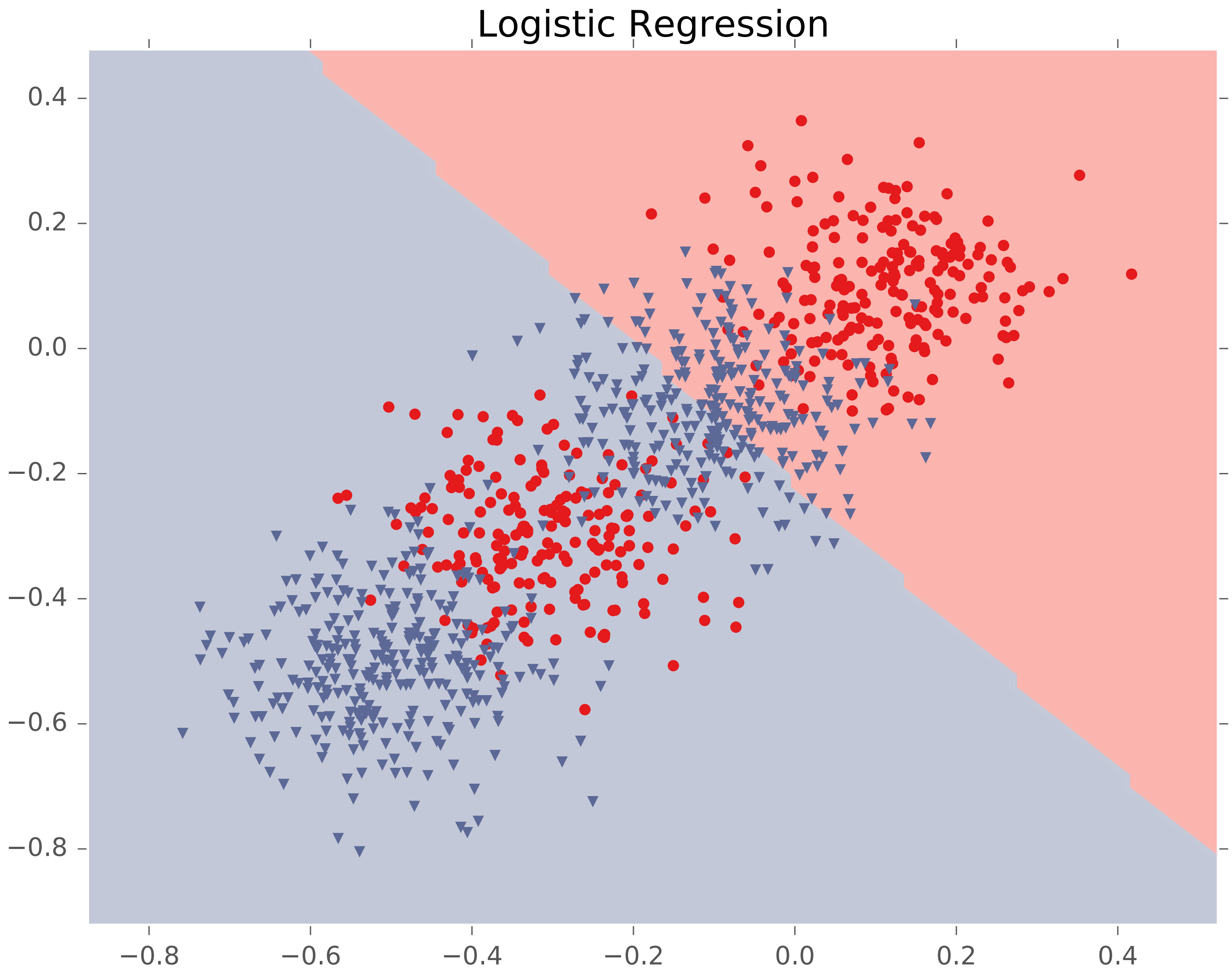

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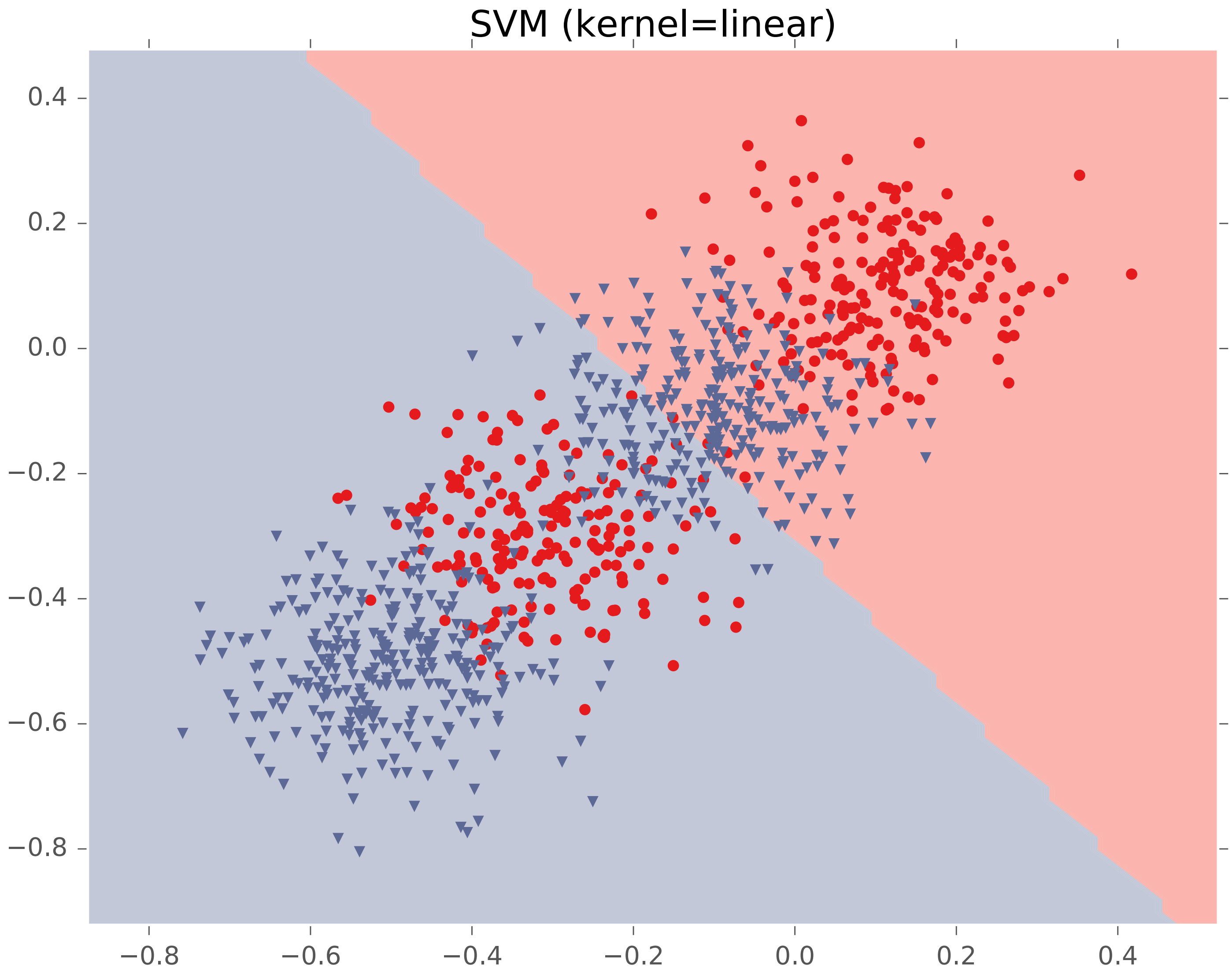

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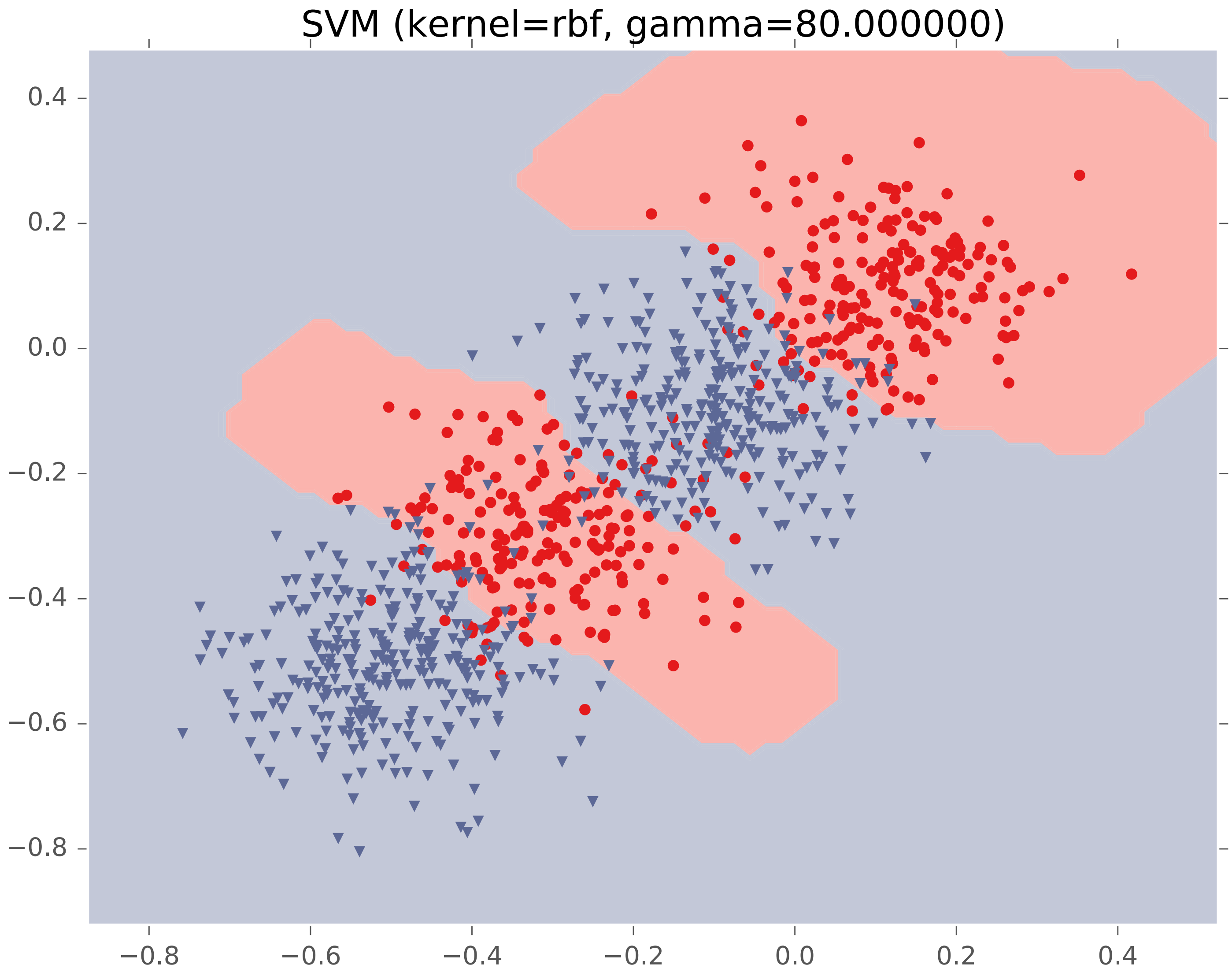

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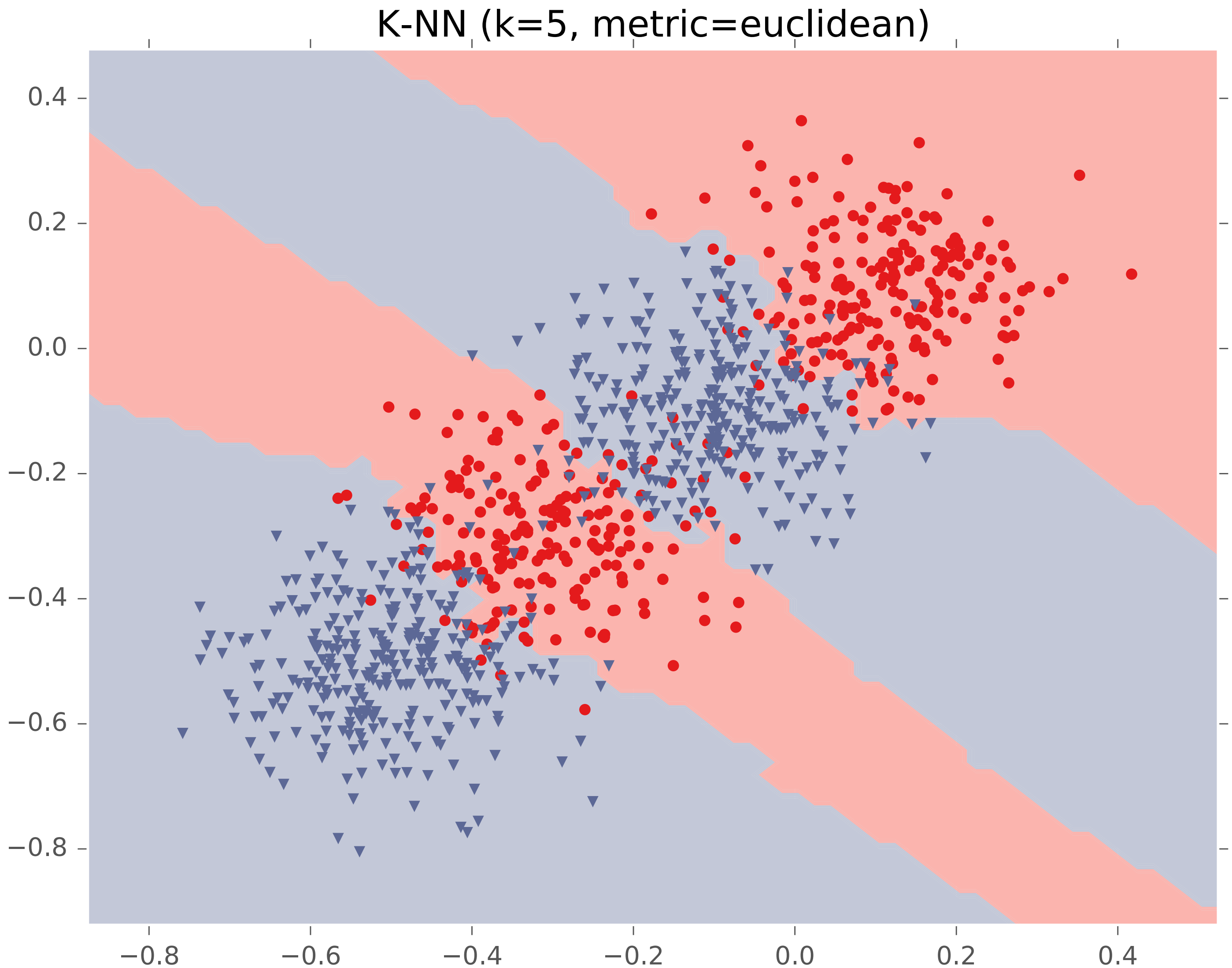

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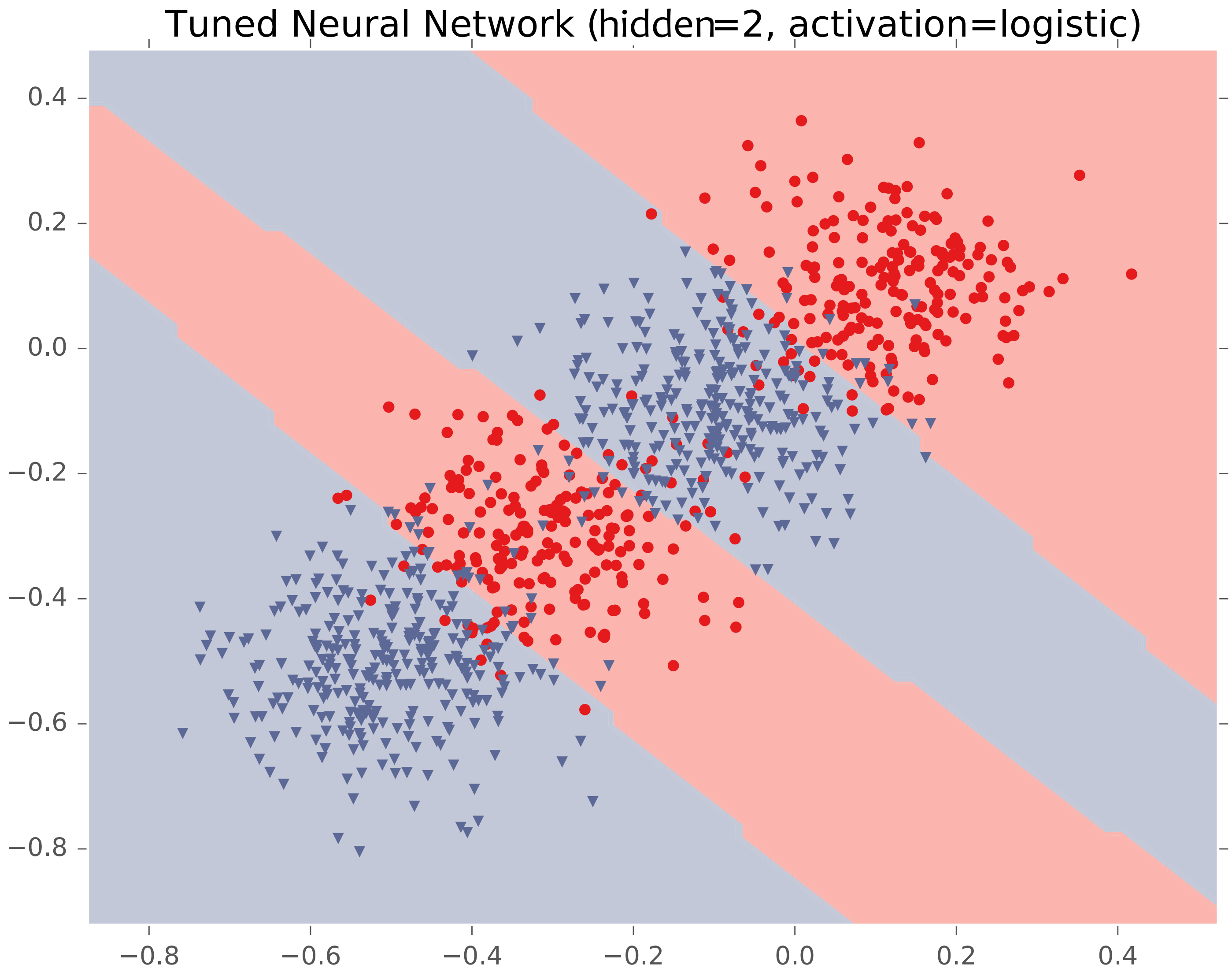

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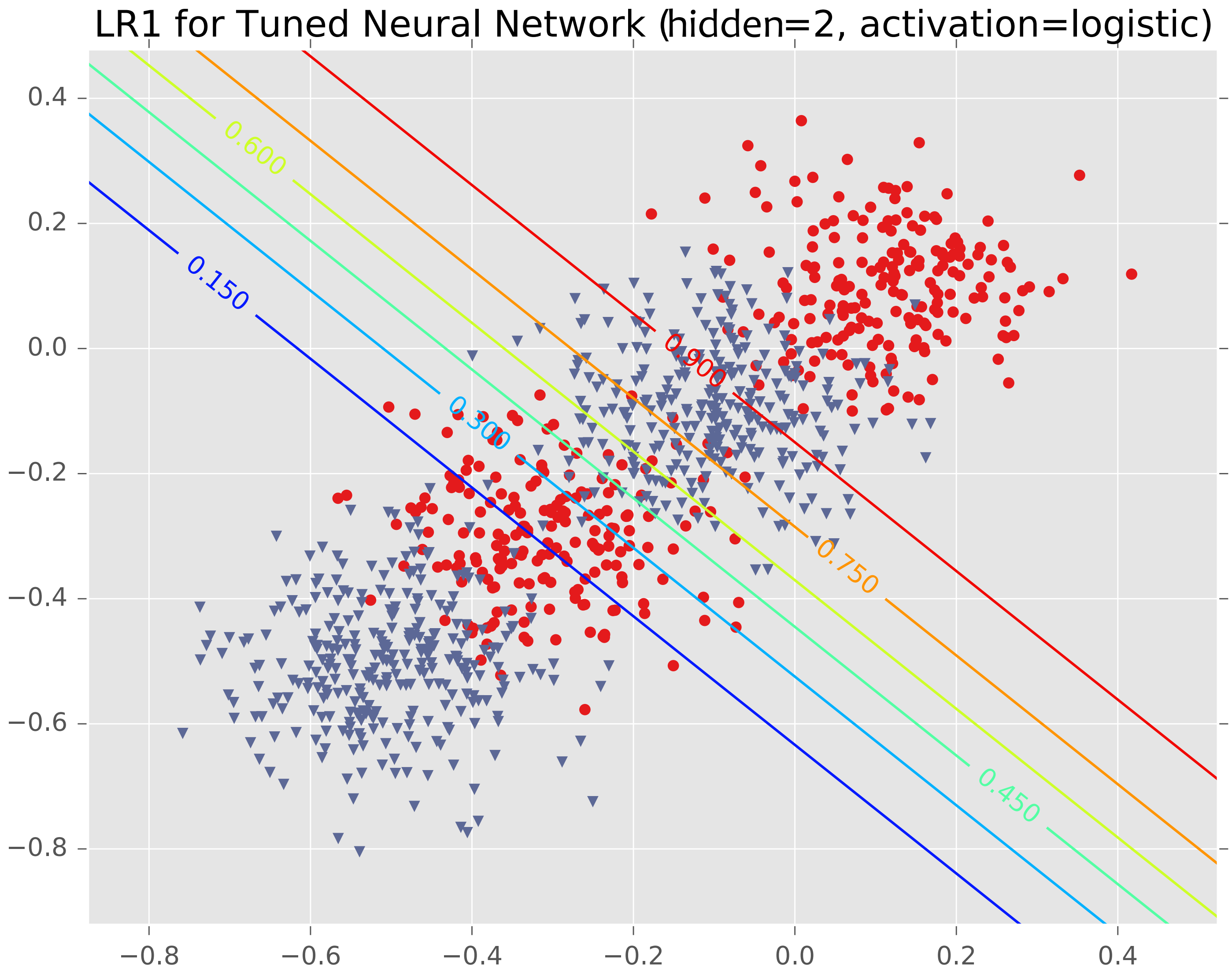

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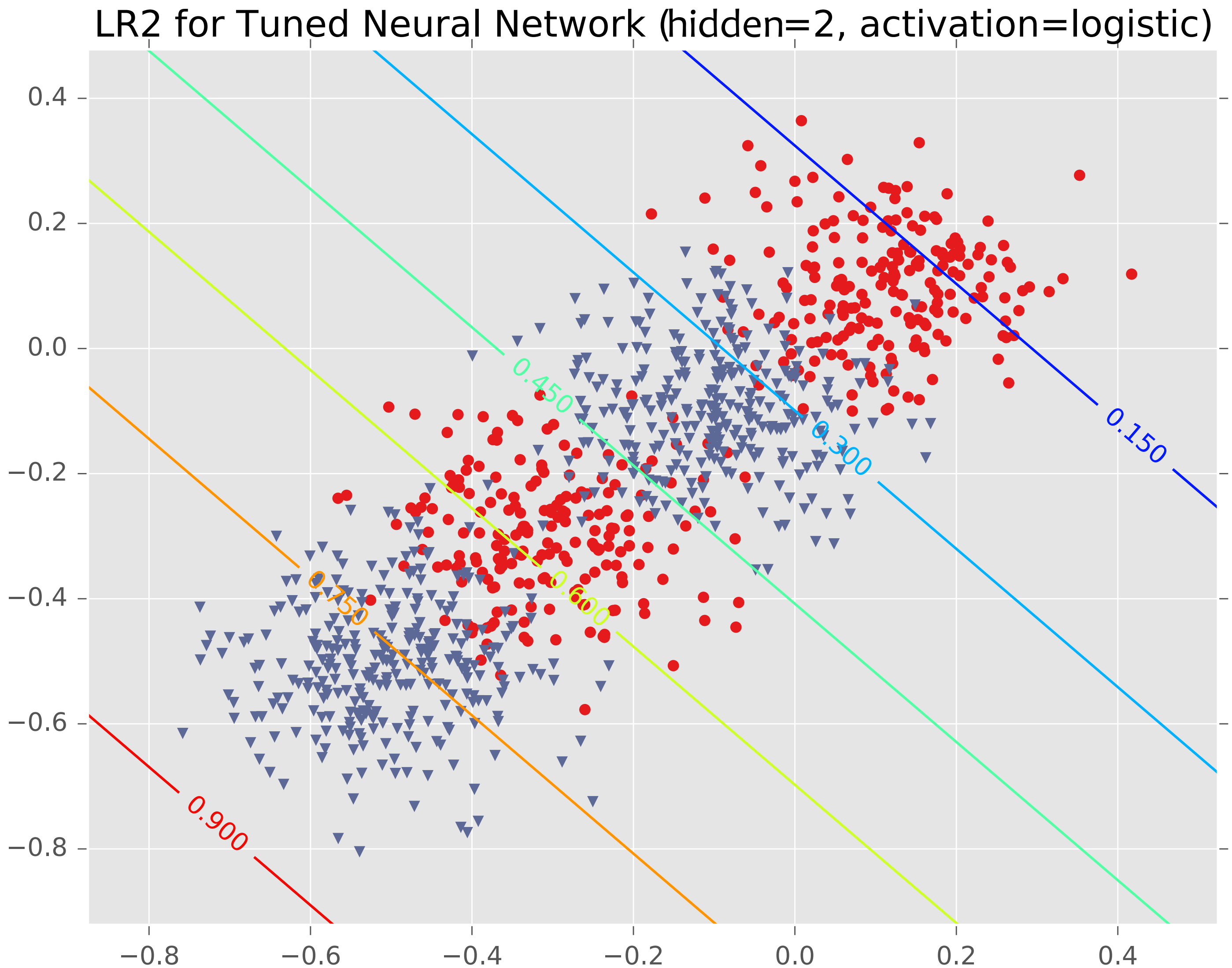

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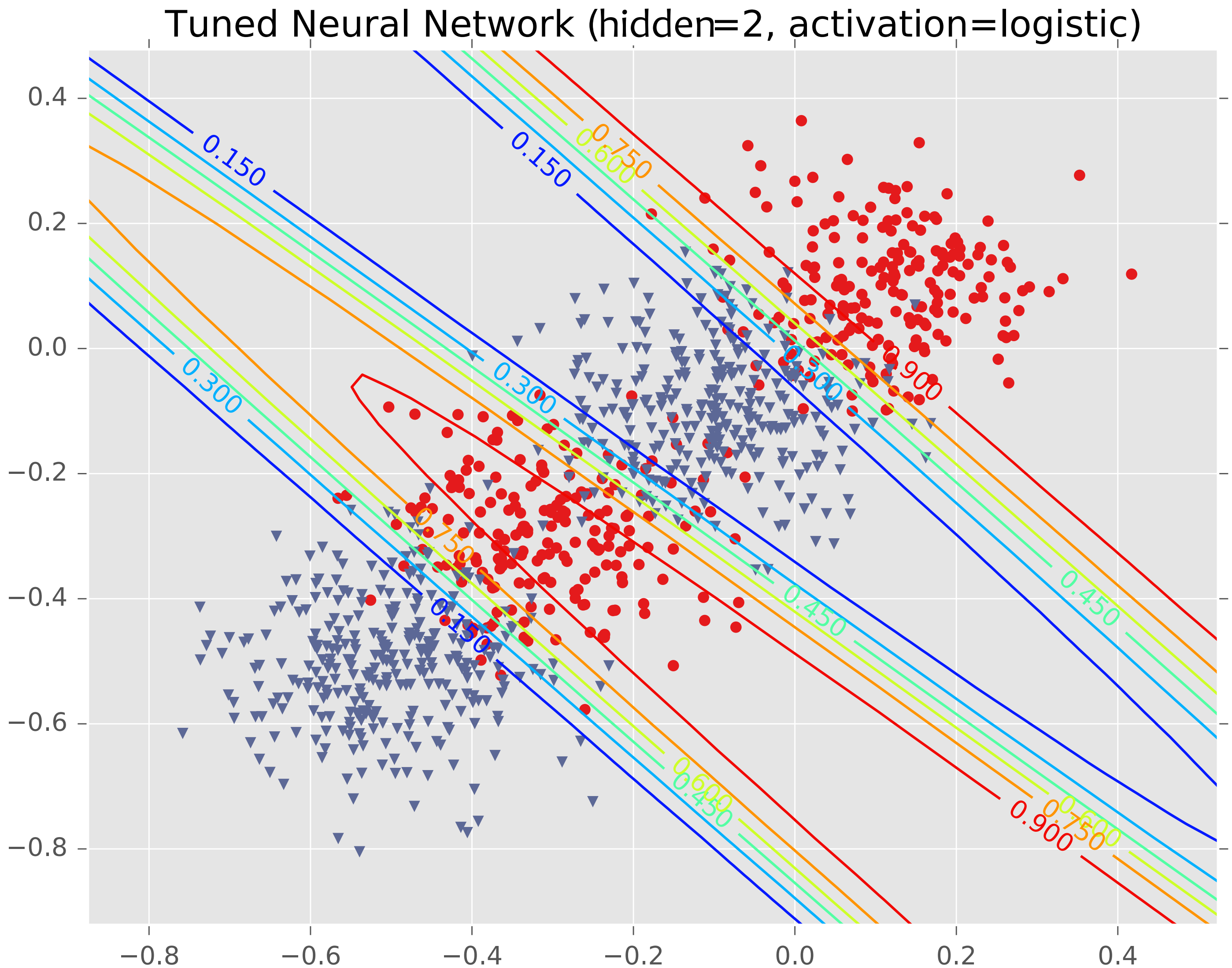

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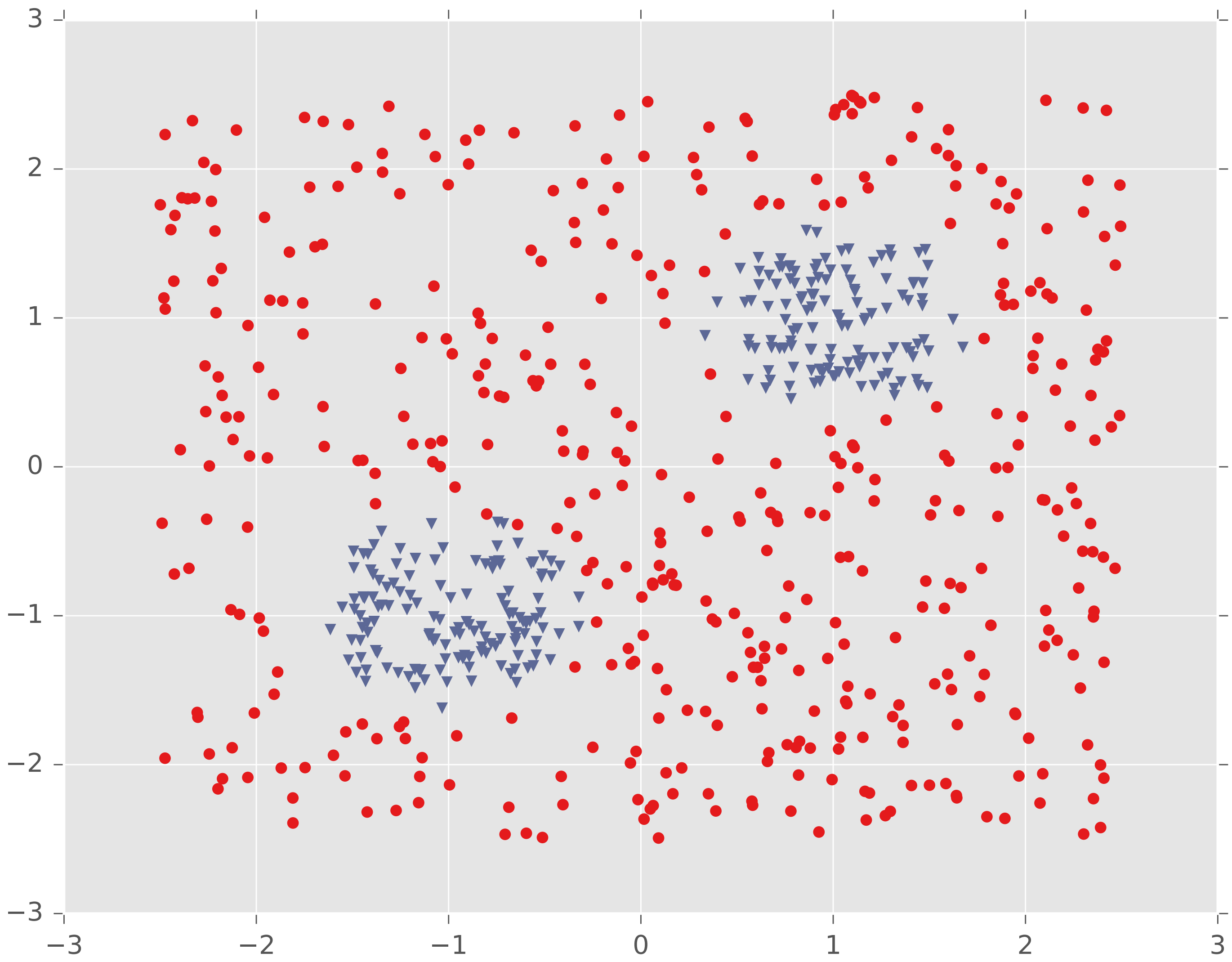

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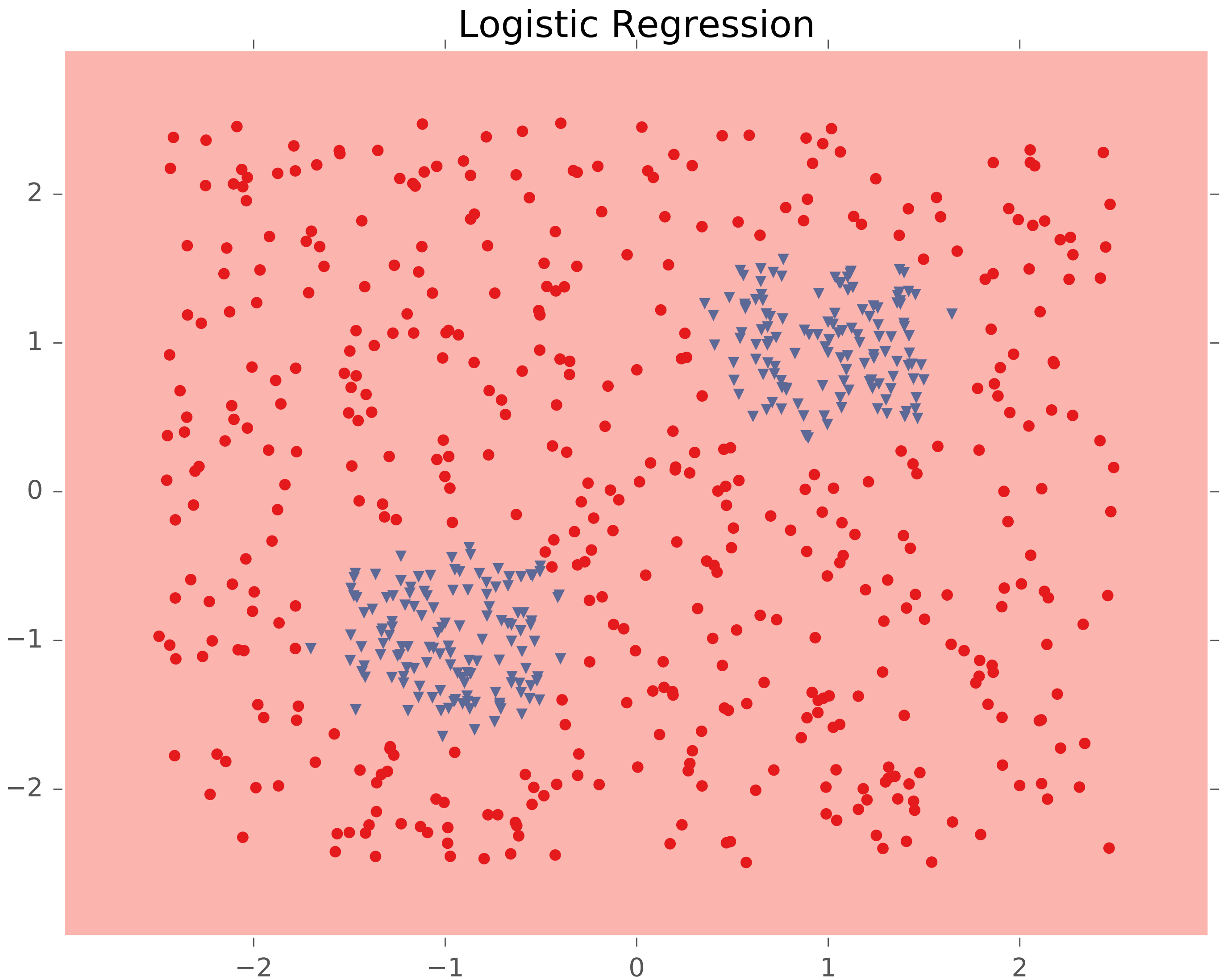

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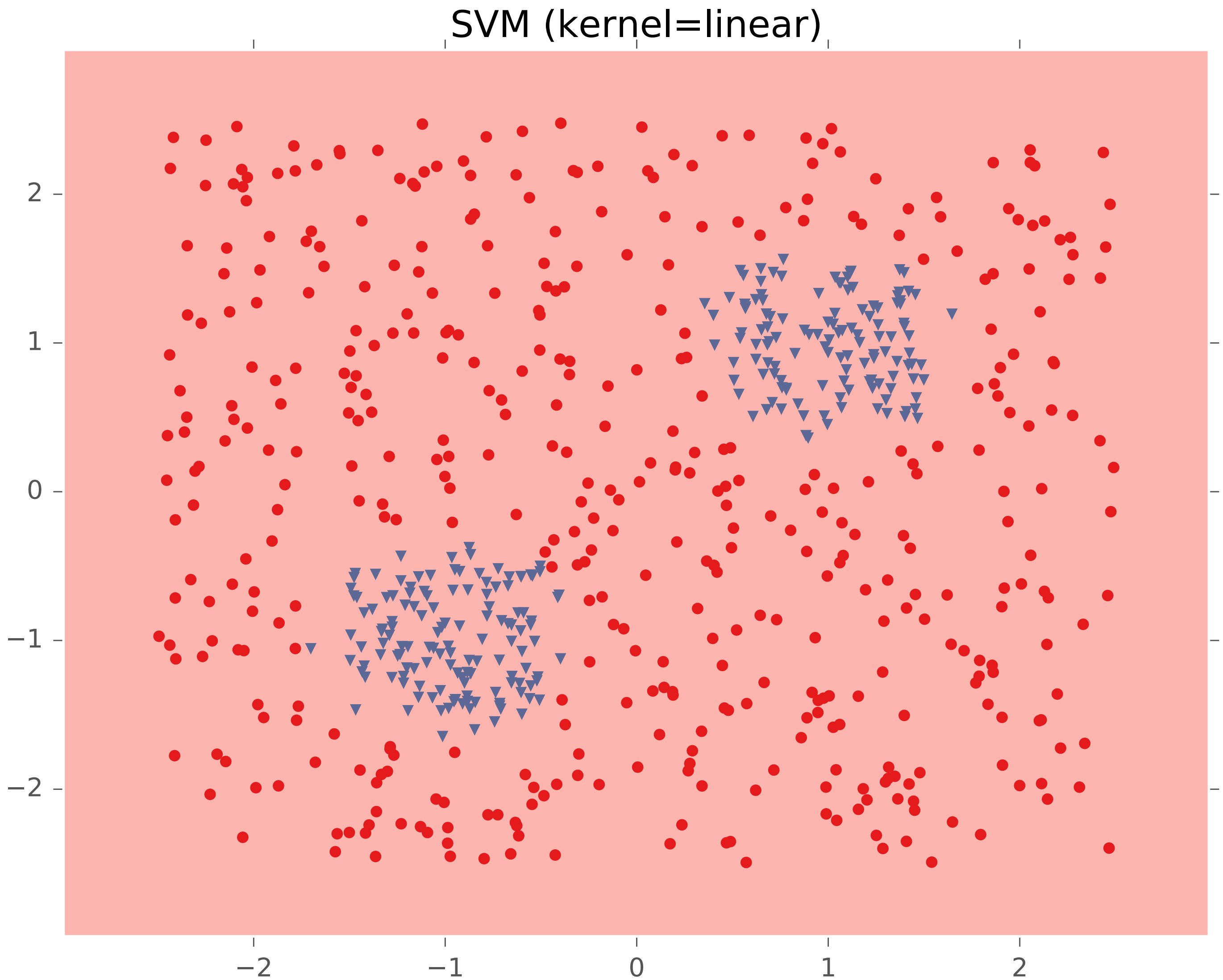

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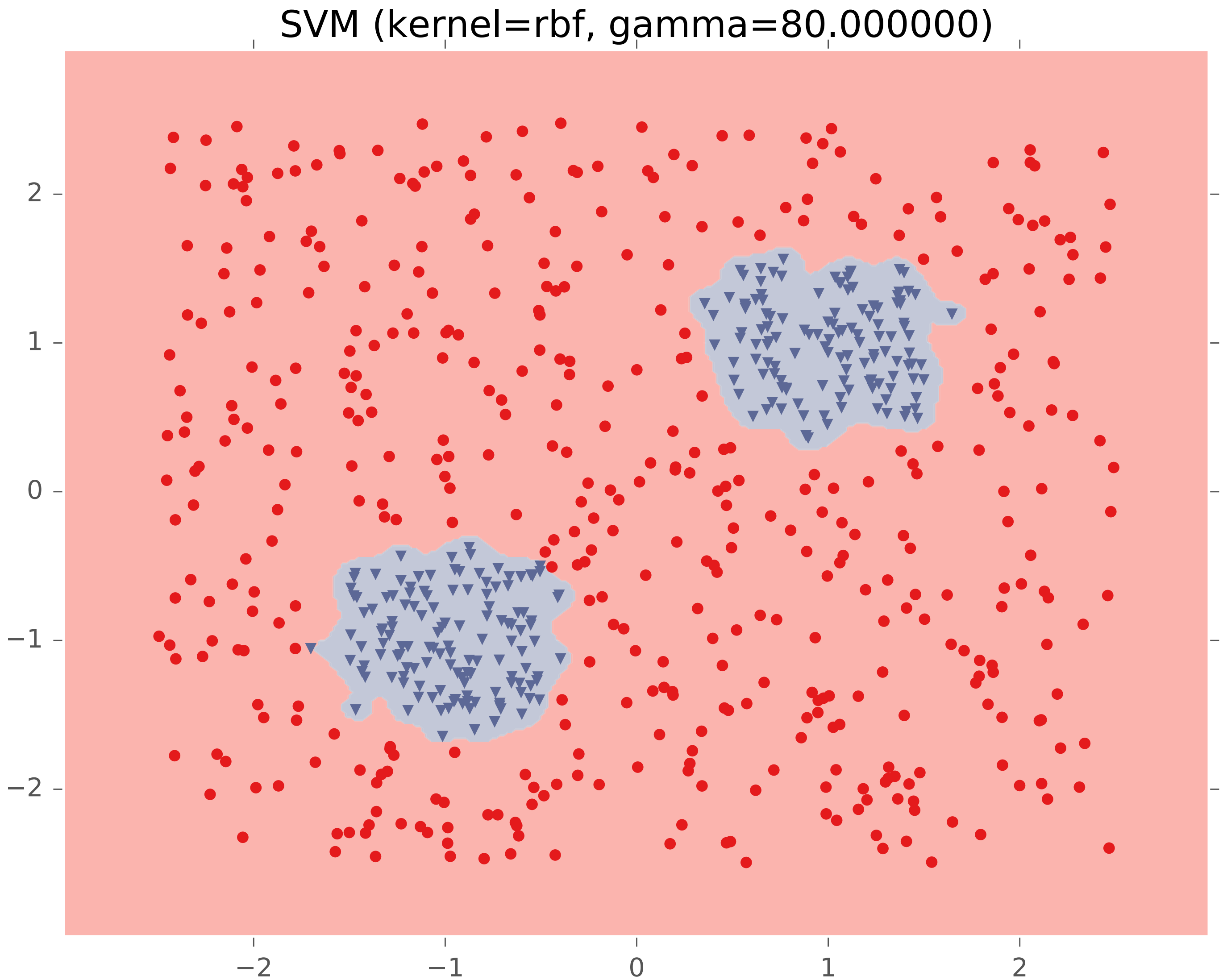

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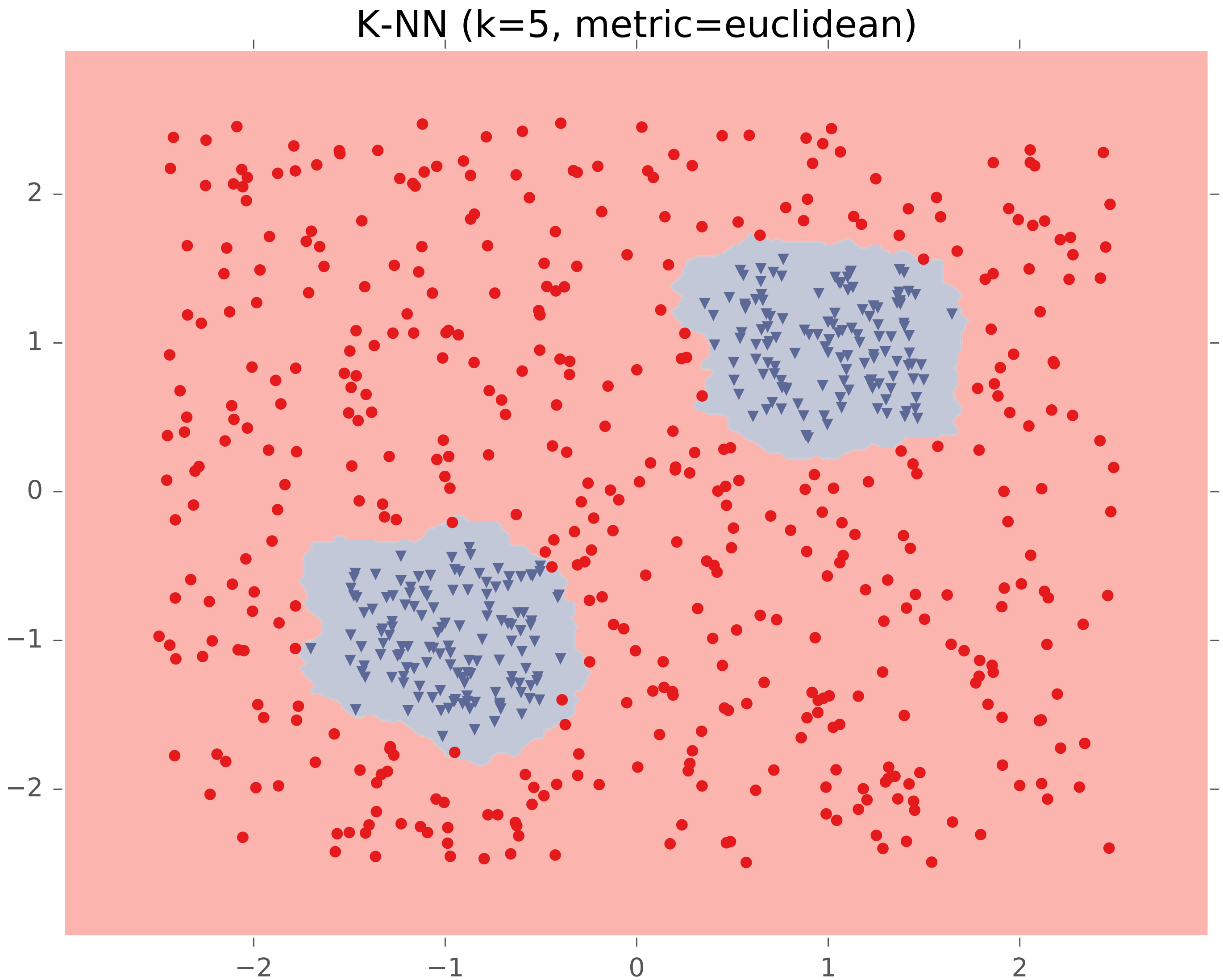

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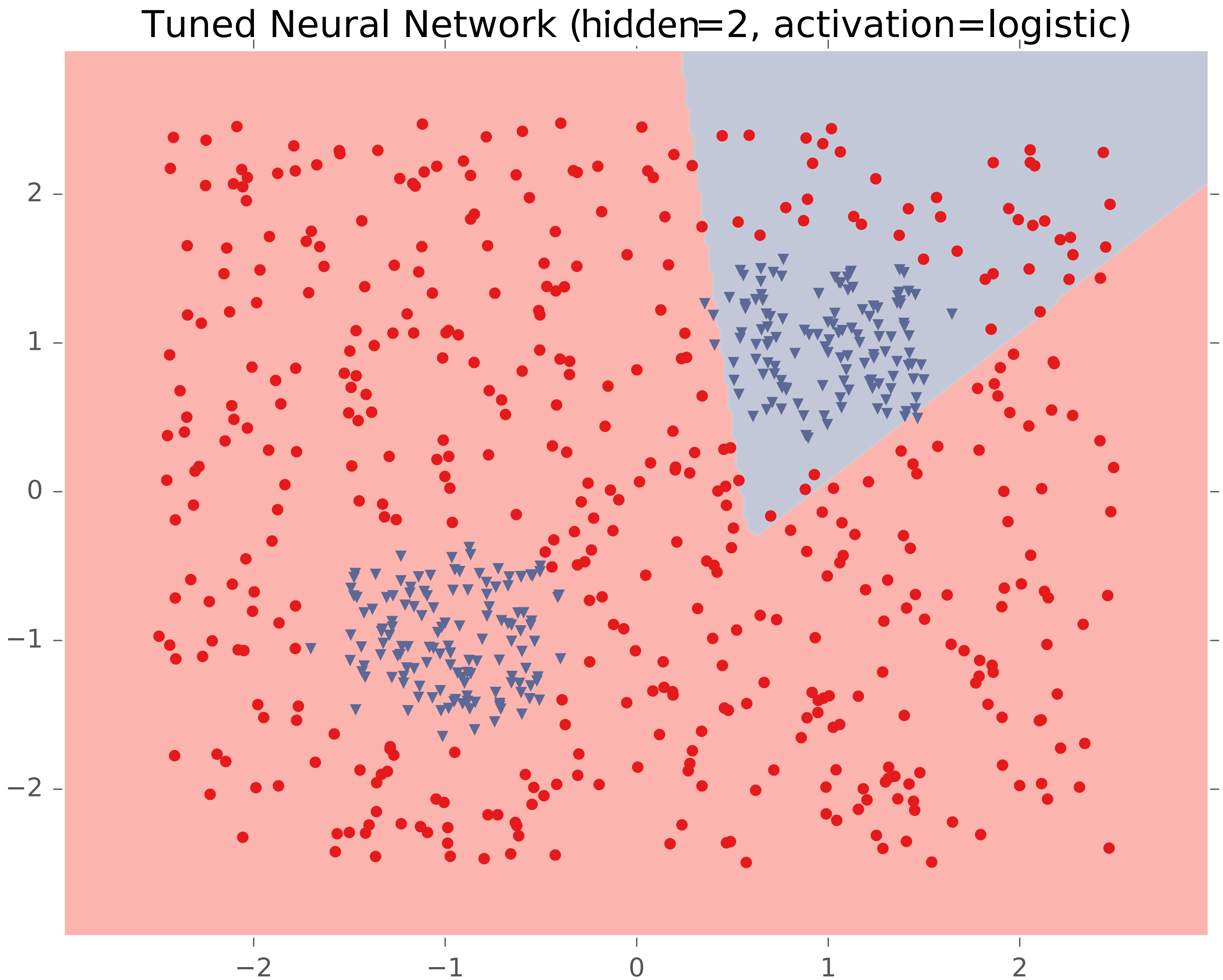

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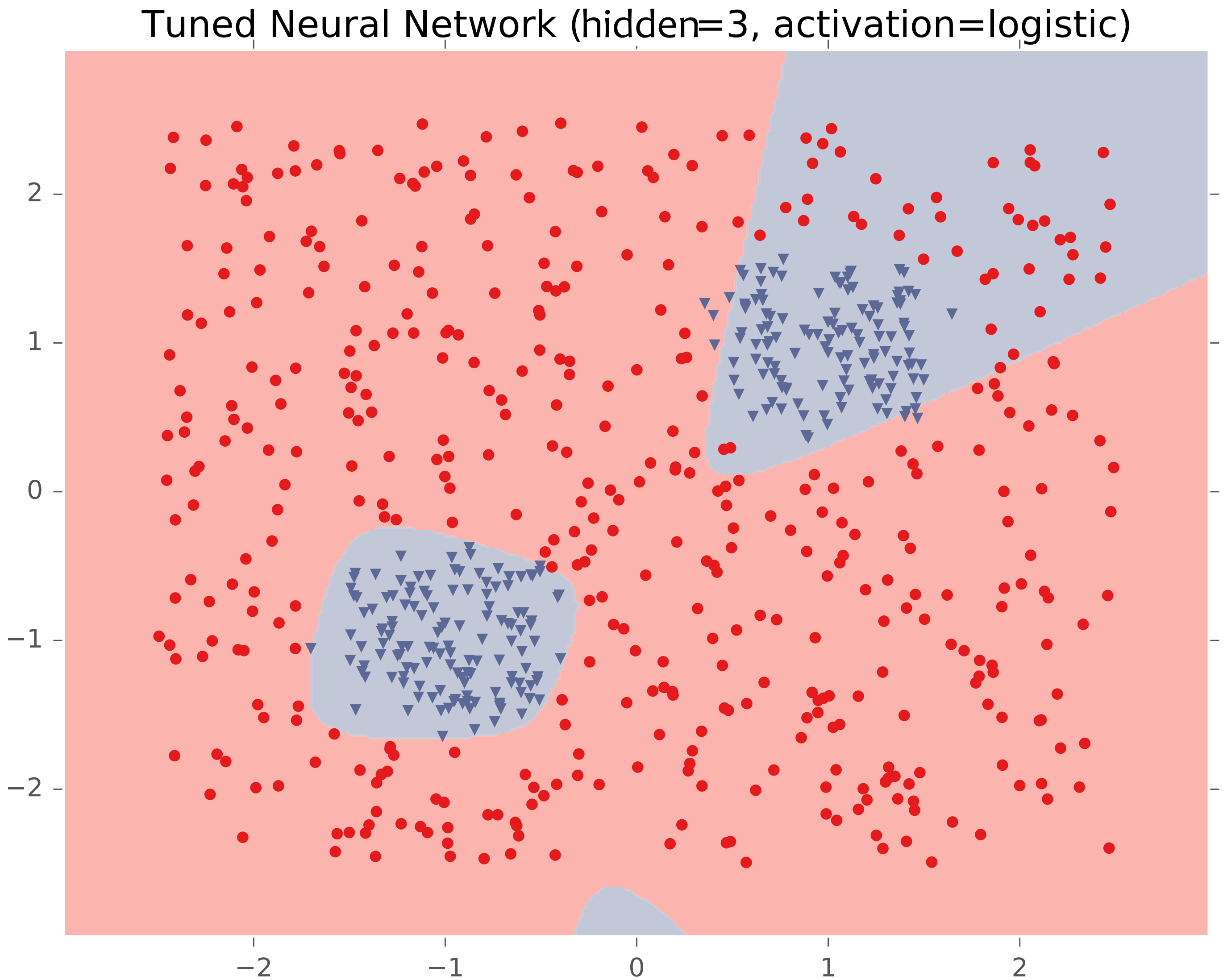

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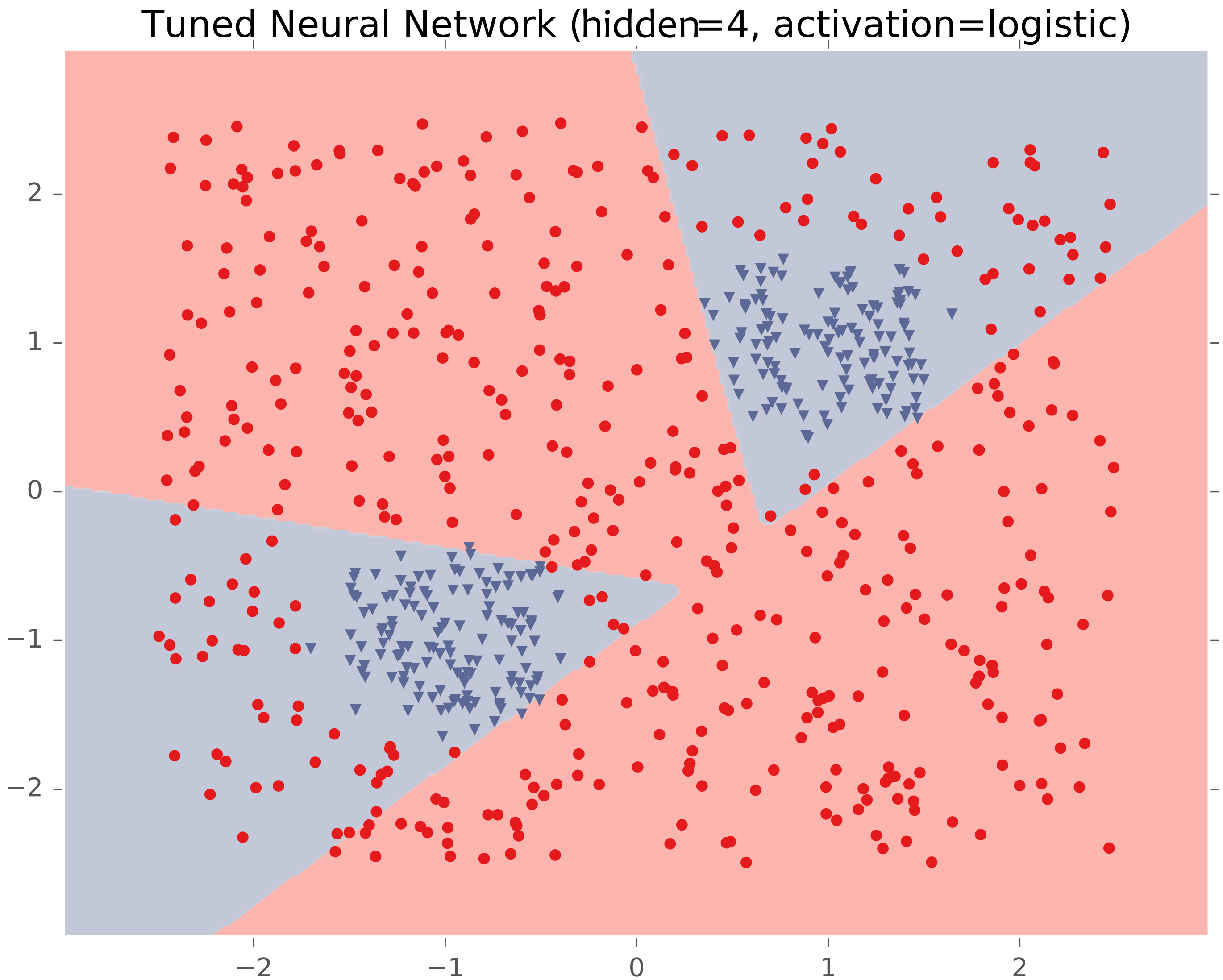

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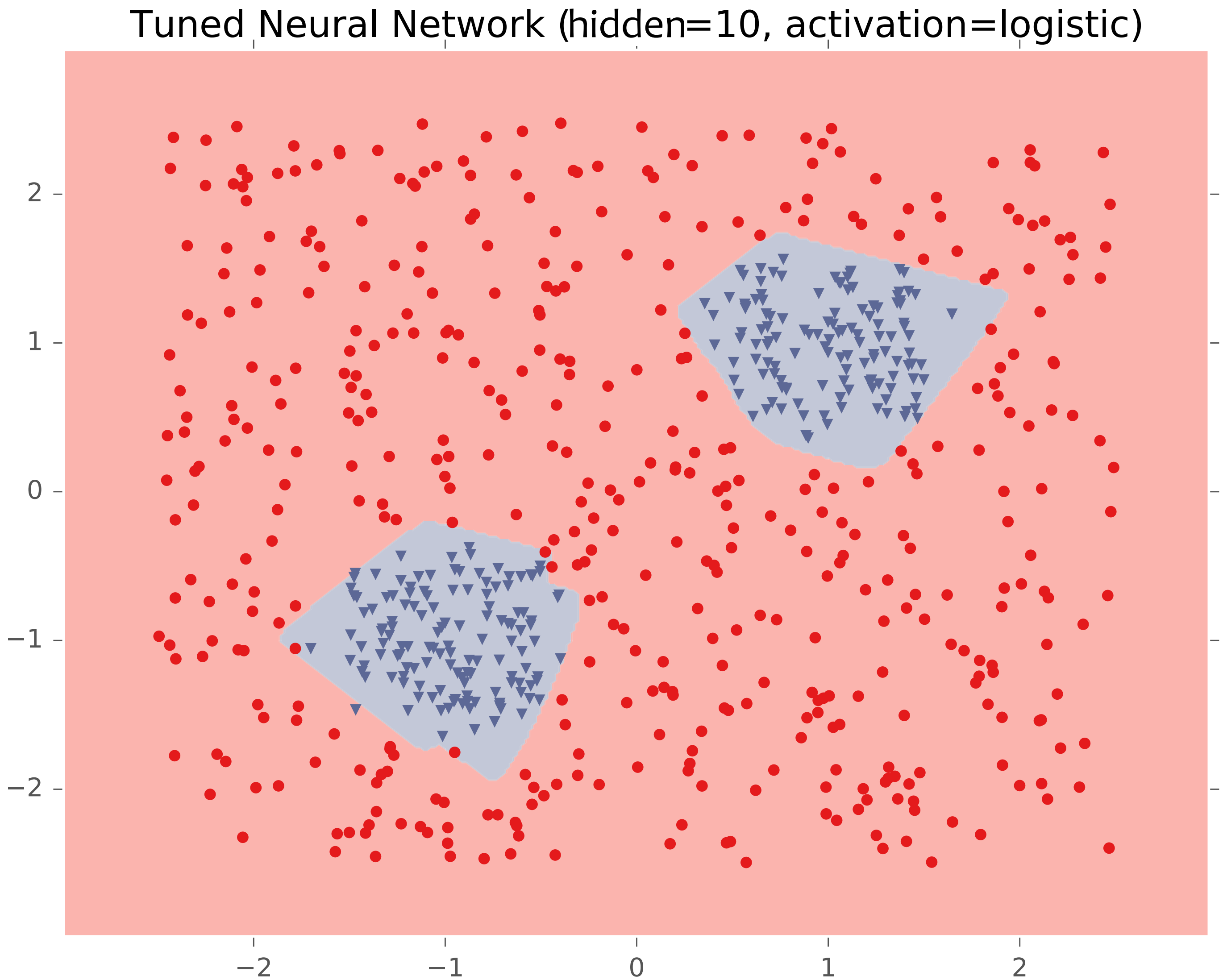


ARCHITECTURES

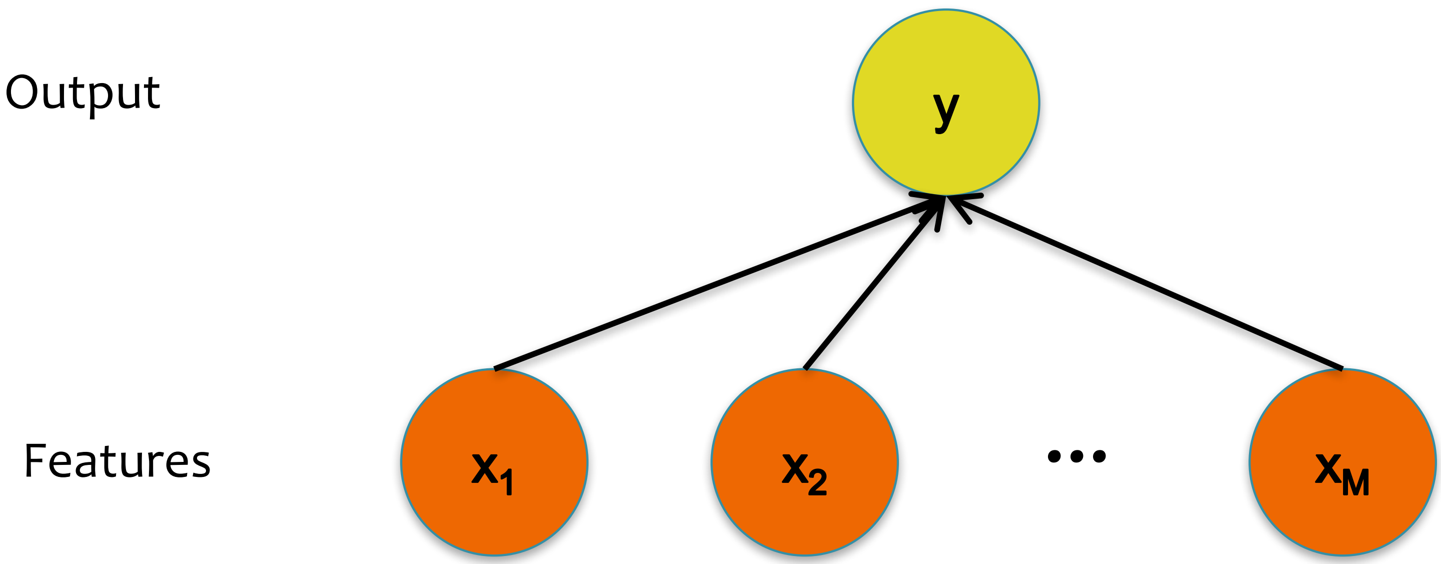
Neural Network Architectures

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

Building a Neural Net

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



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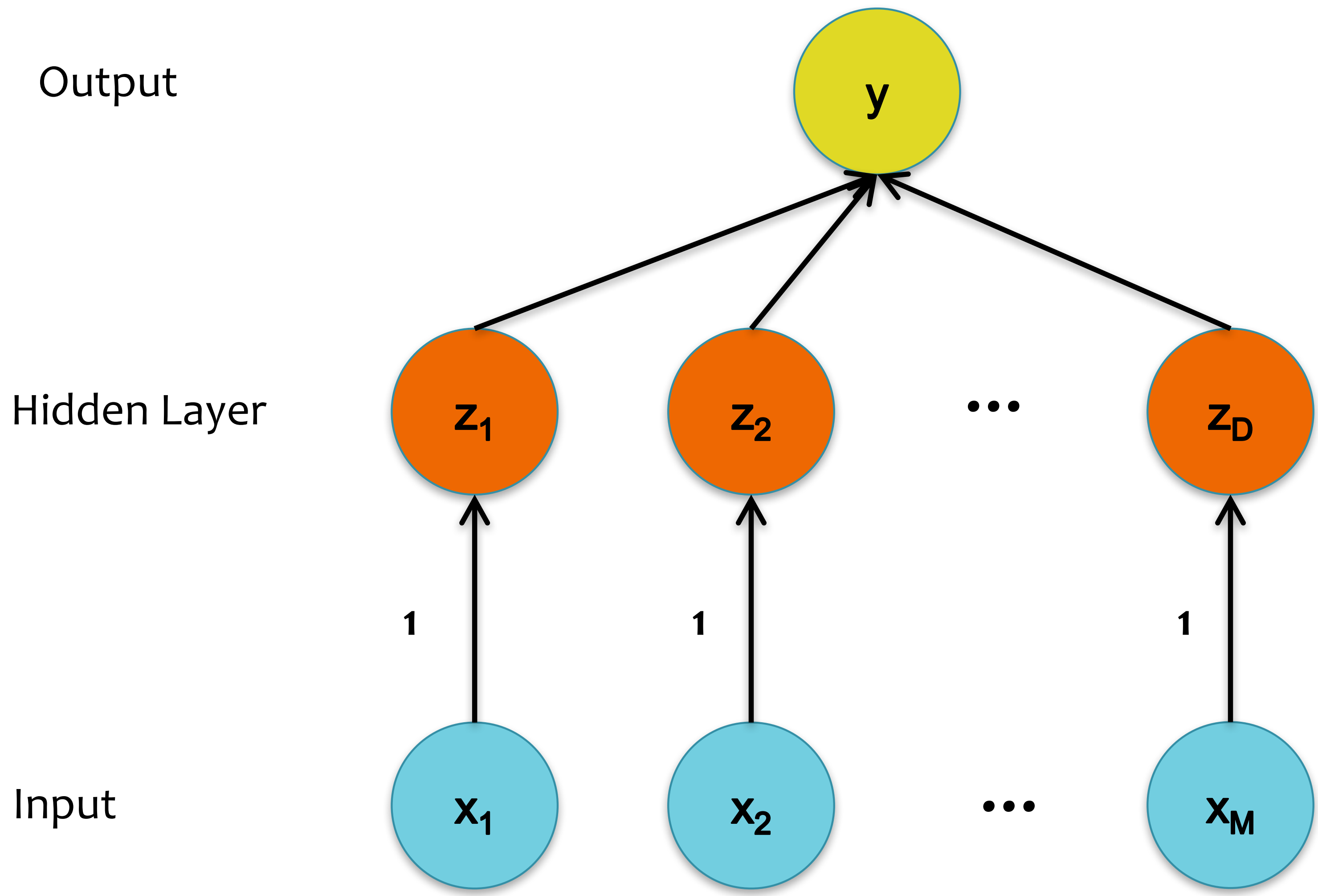

D = M

Building a Neural Net

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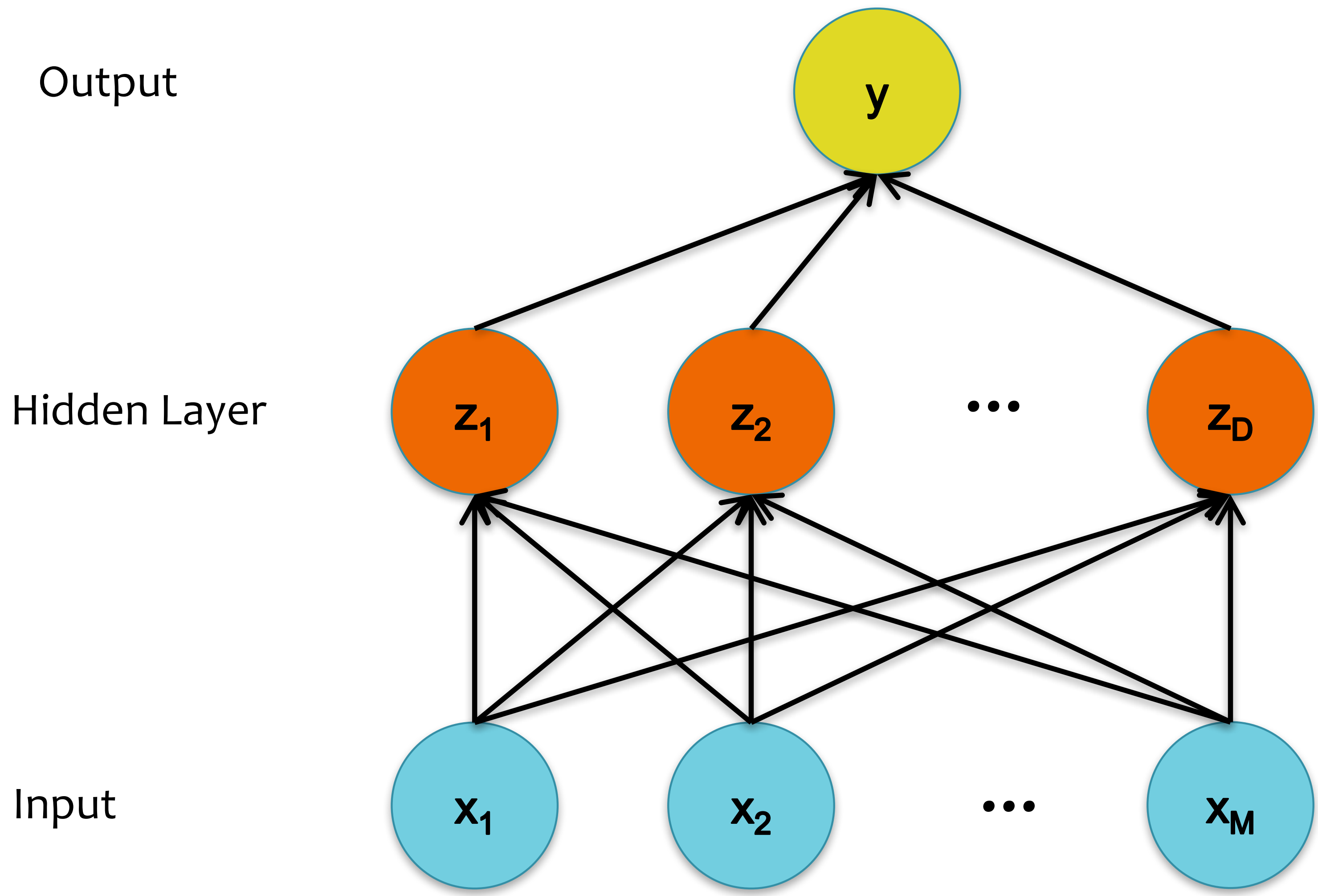

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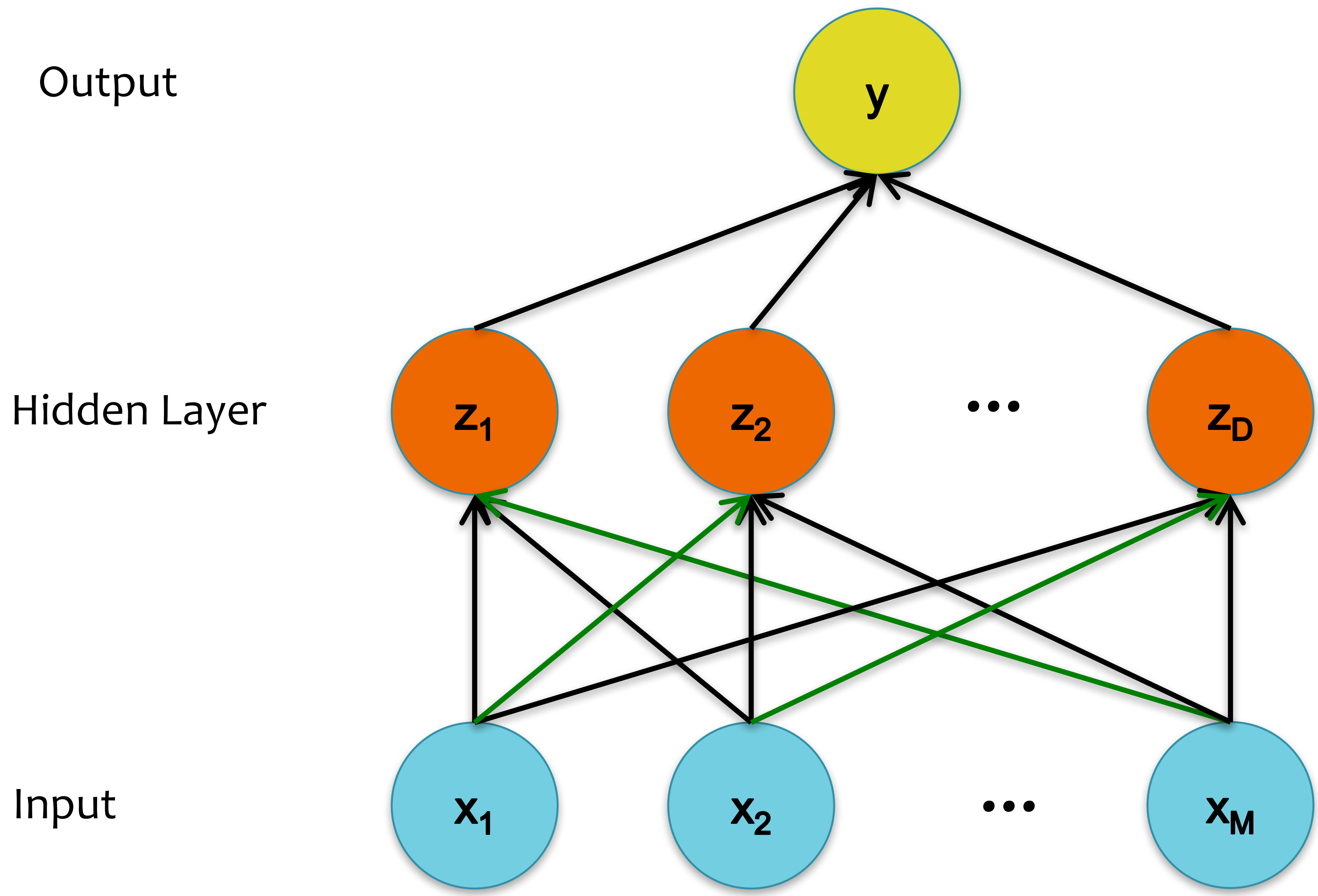

D = M

Building a Neural Net

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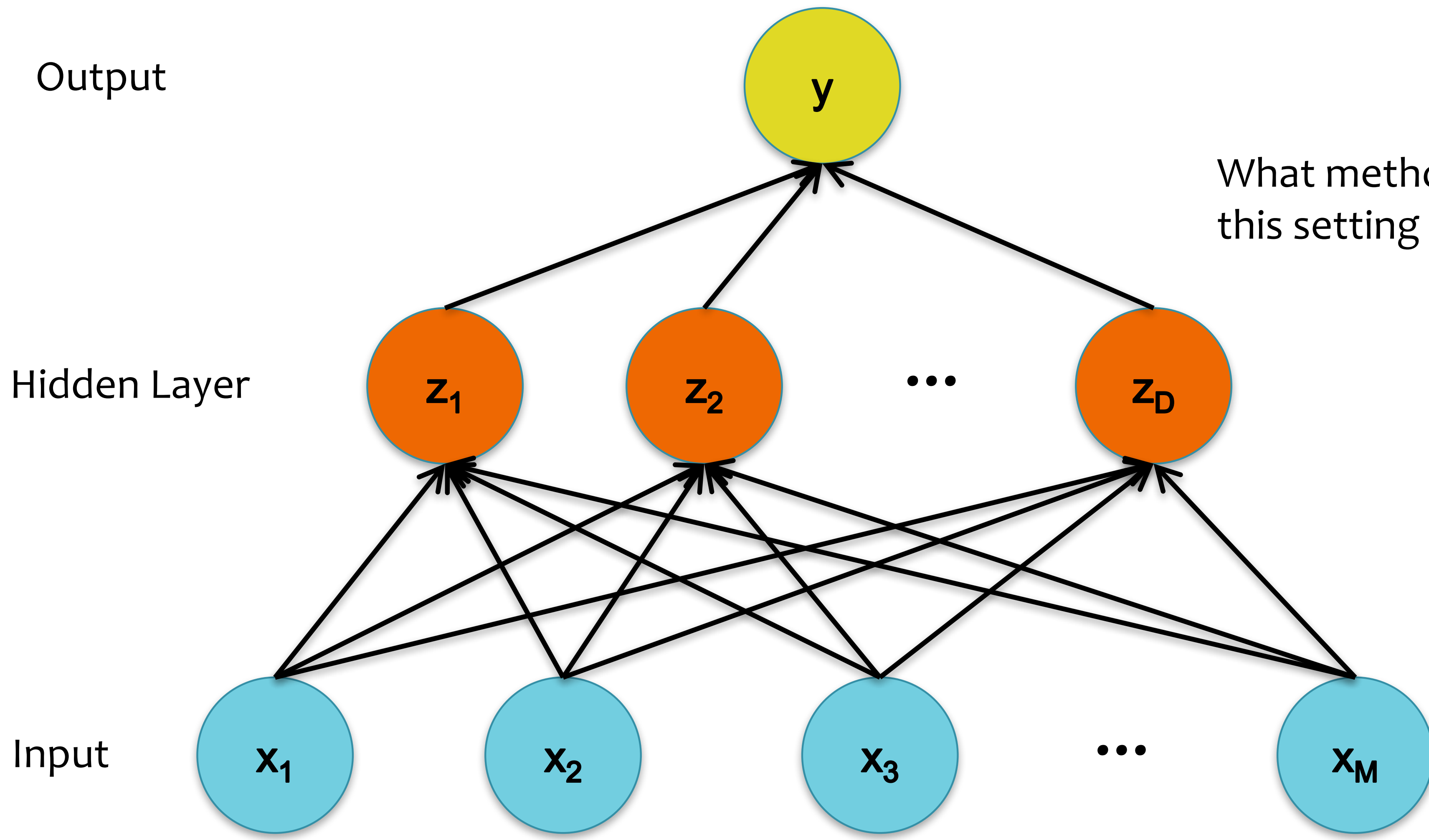
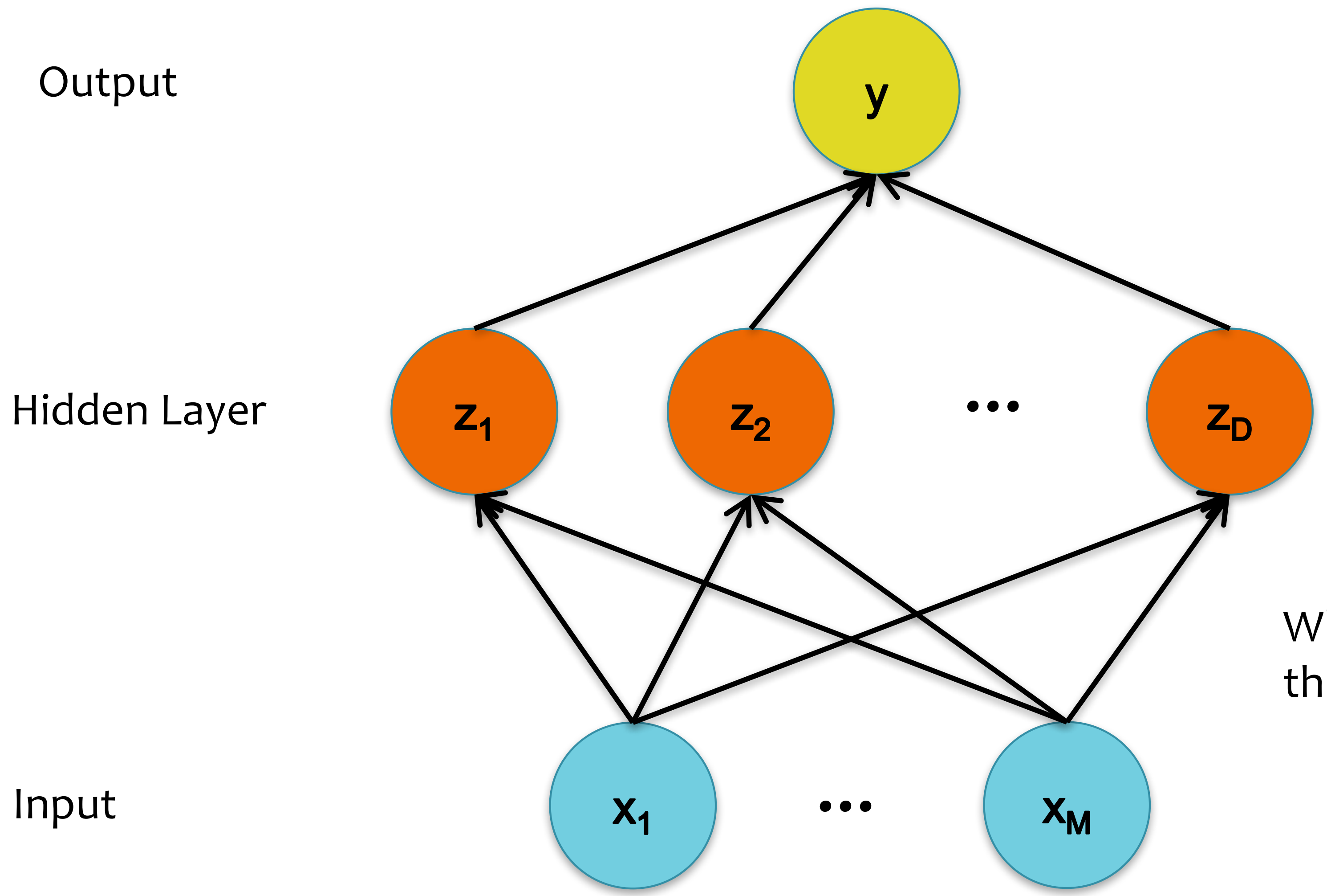


What method(s) is this setting similar to?

D < M

Building a Neural Net

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



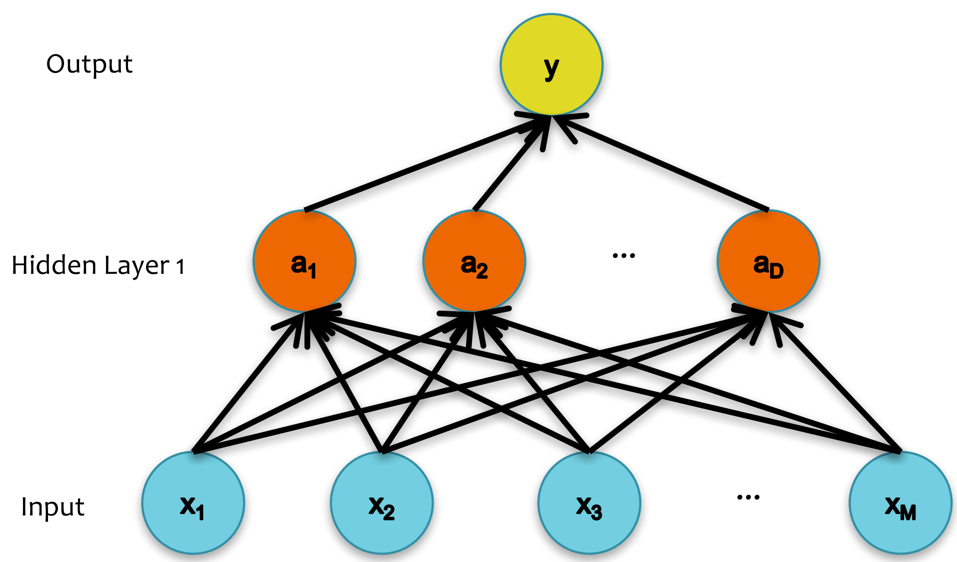
D > M

What method(s) is
this setting similar to?

Decision Functions

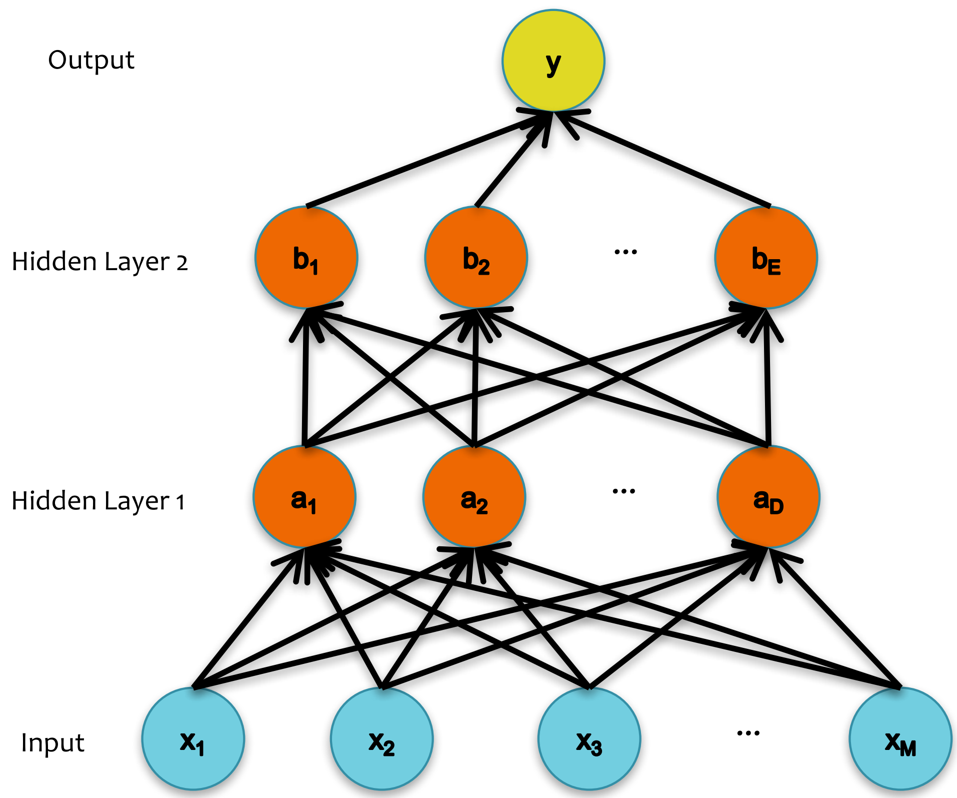
Deeper Networks

Q: How many layers should we use?



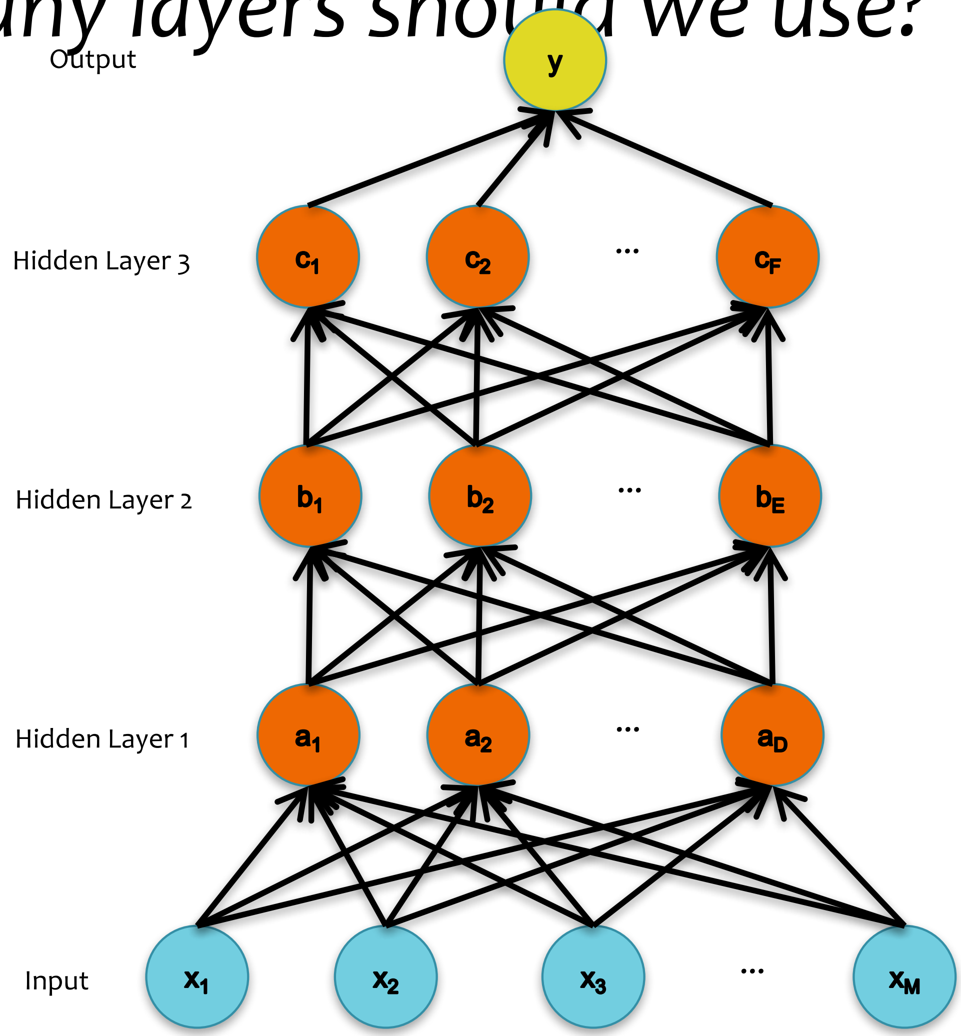
Deeper Networks

Q: How many layers should we use?



Deeper Networks

Q: How many layers should we use?



Deeper Networks

Q: How many layers should we use?

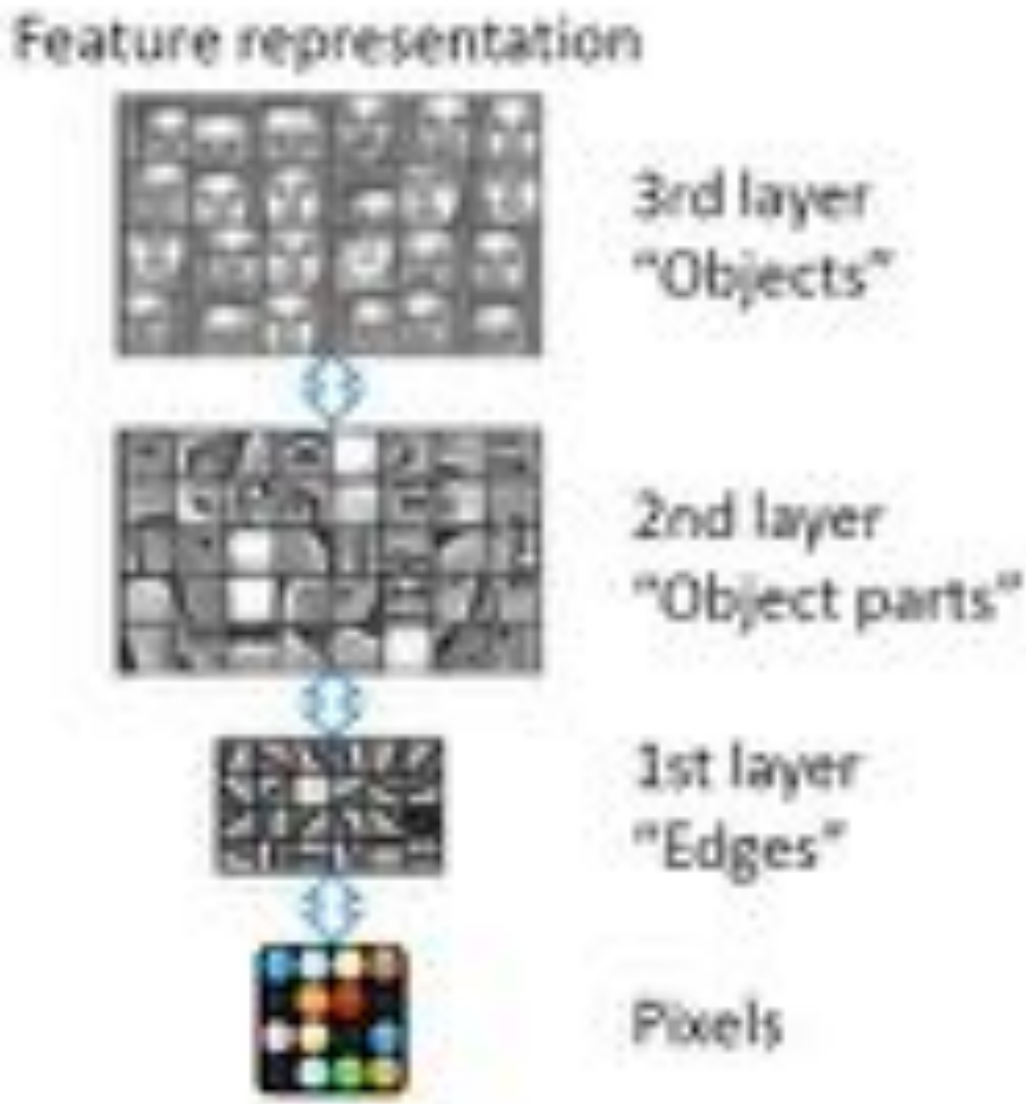
- **Theoretical answer:**
  - A neural network with 1 hidden layer is a **universal function approximator**
  - Cybenko (1989): For any continuous function g(**x**), there exists a 1-hidden-layer neural net $h_\theta(\mathbf{x})$ s.t. $| h_\theta(\mathbf{x}) - g(\mathbf{x}) | < \epsilon$ for all **x**, 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.

Decision Functions

Different Levels of Abstraction

- We don’t know the “right” levels of abstraction
- So let the model figure it out!



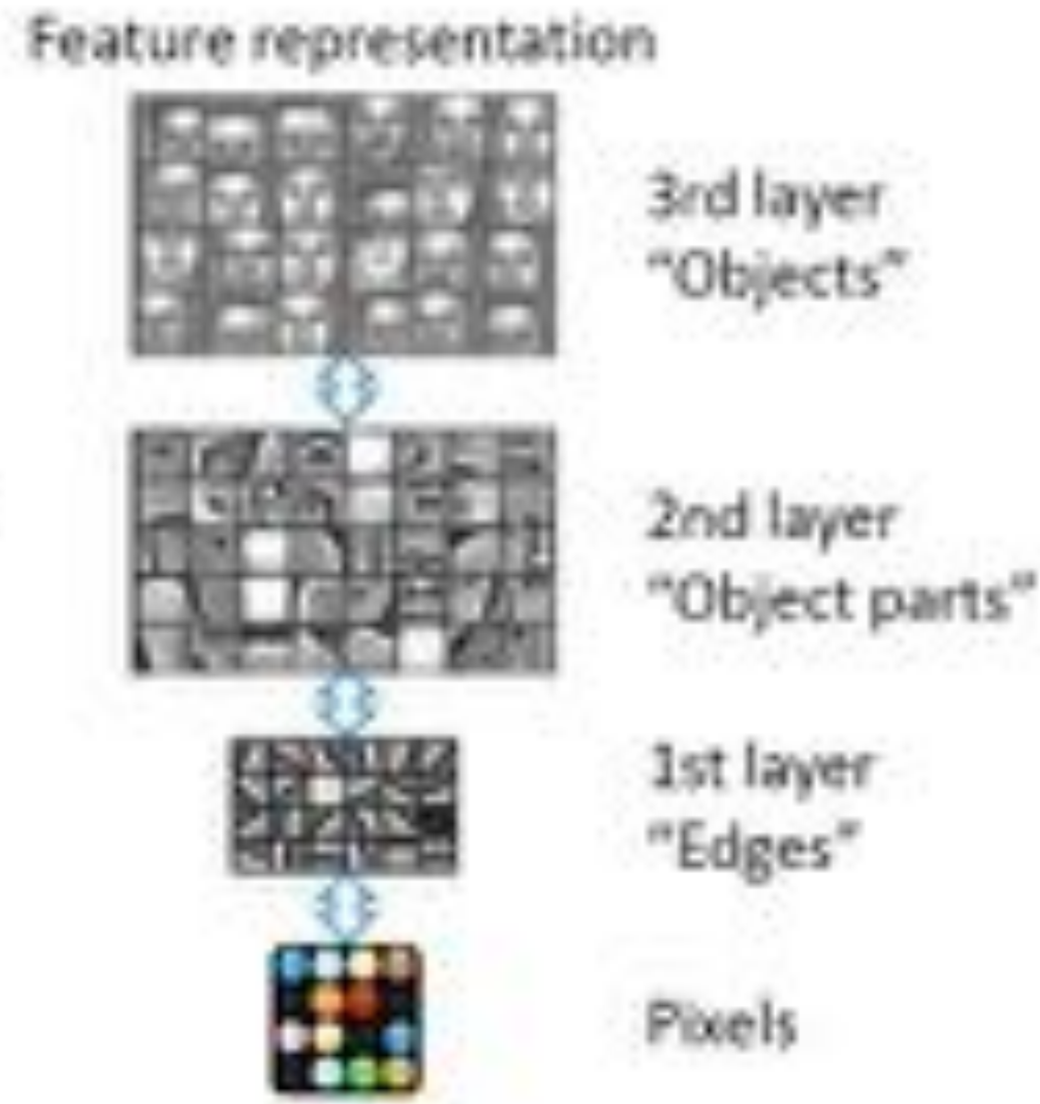
Example from Honglak Lee (NIPS 2010)

Decision Functions

Different Levels of Abstraction

Face Recognition:

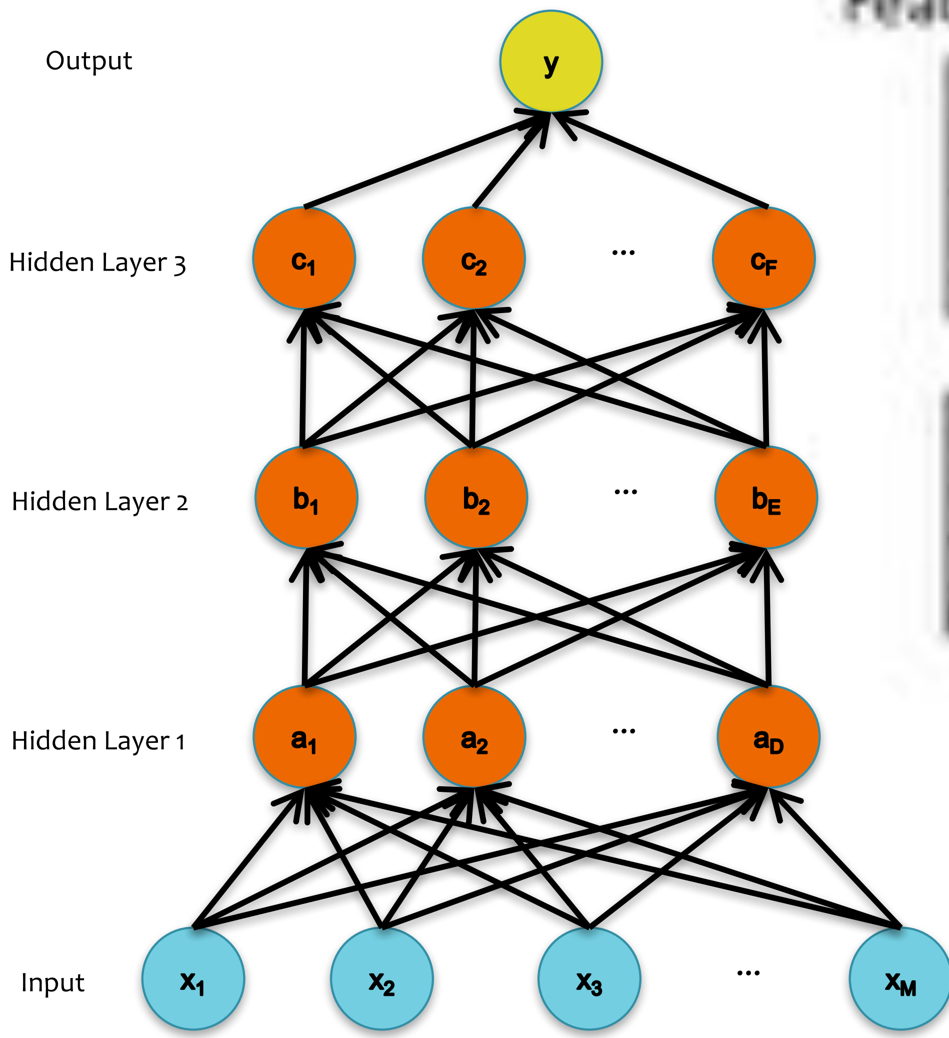
- Deep Network can build up increasingly higher levels of abstraction
- Lines, parts, regions

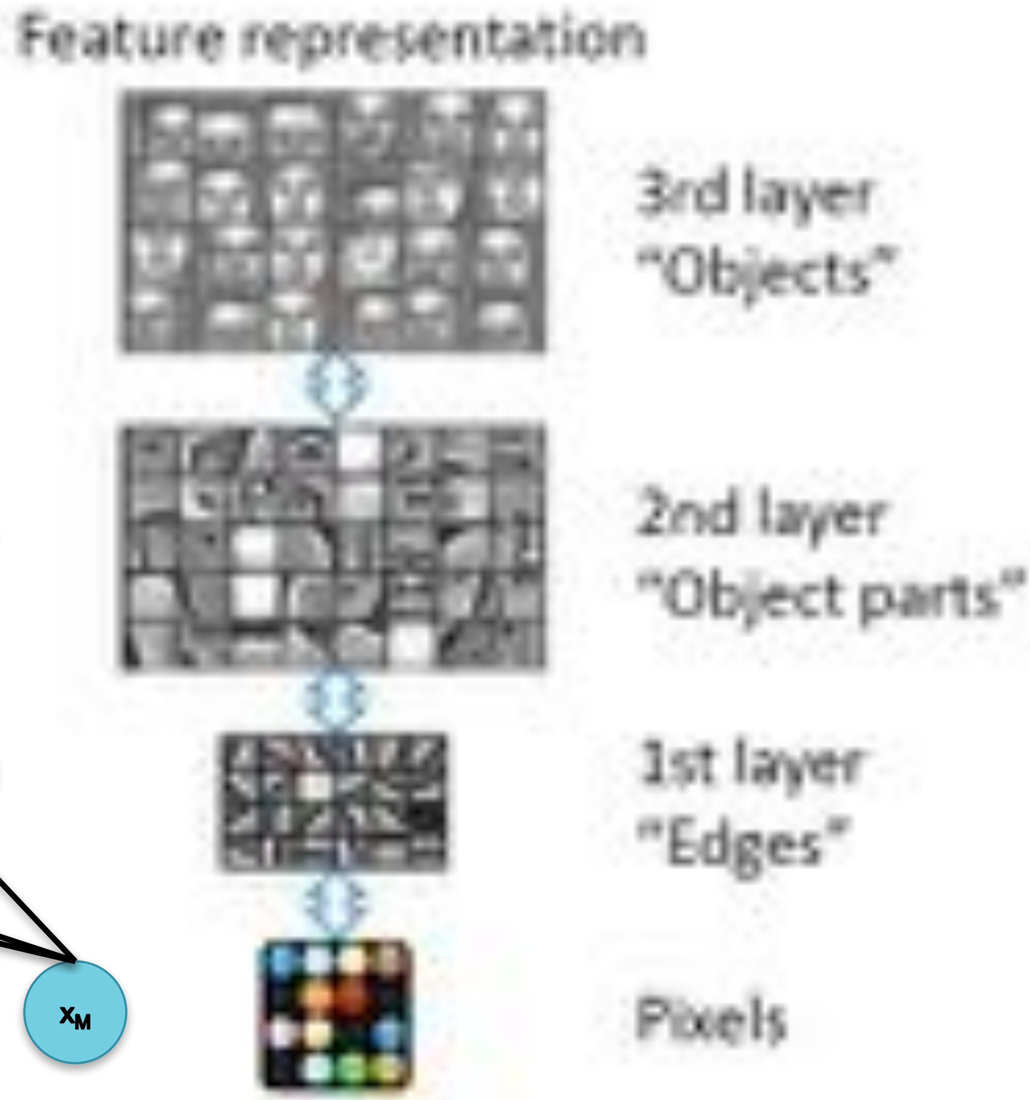


Example from Honglak Lee (NIPS 2010)

Decision Functions

Different Levels of Abstraction

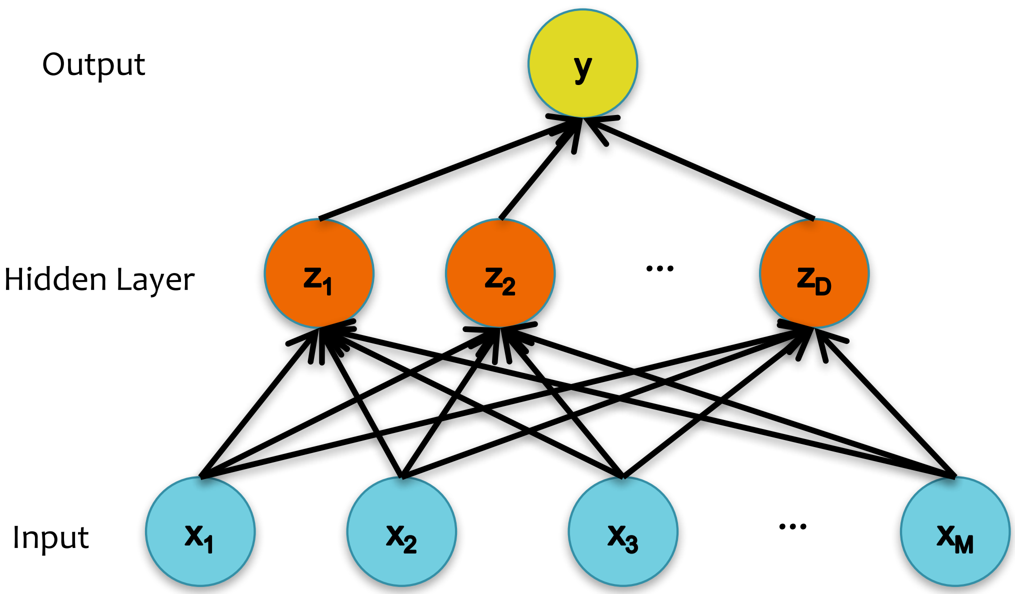


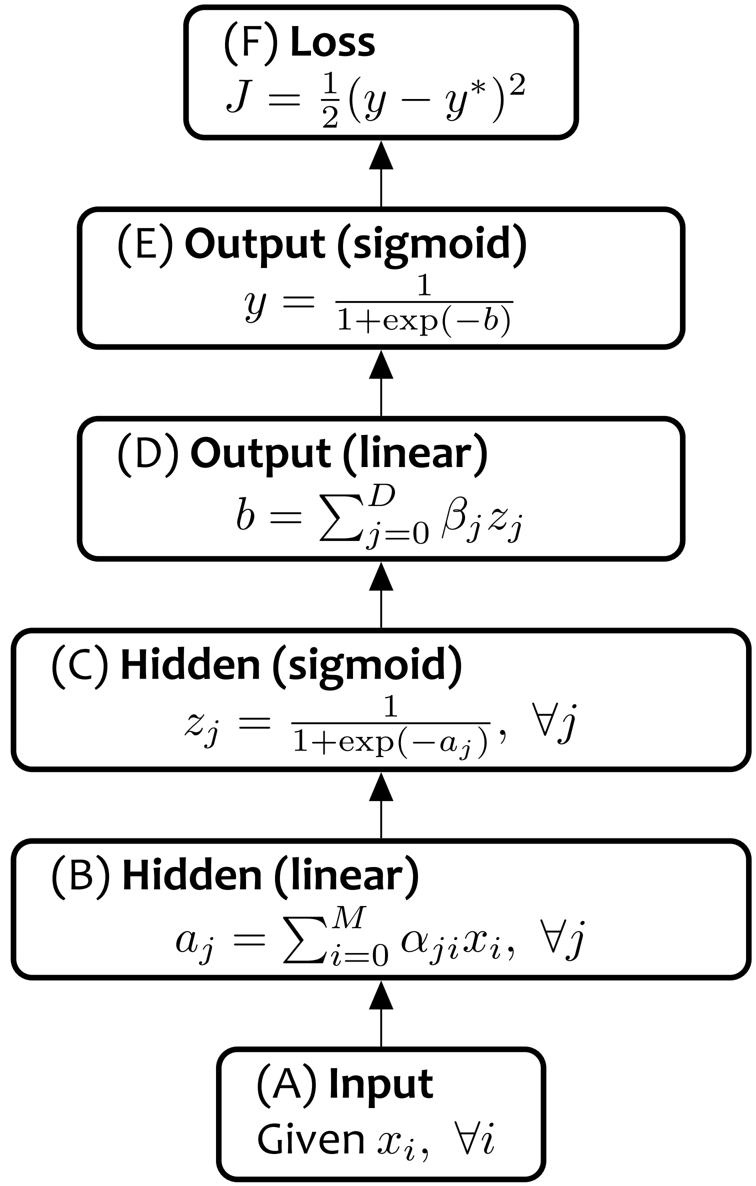


Example from Honglak Lee (NIPS 2010)

Activation Functions

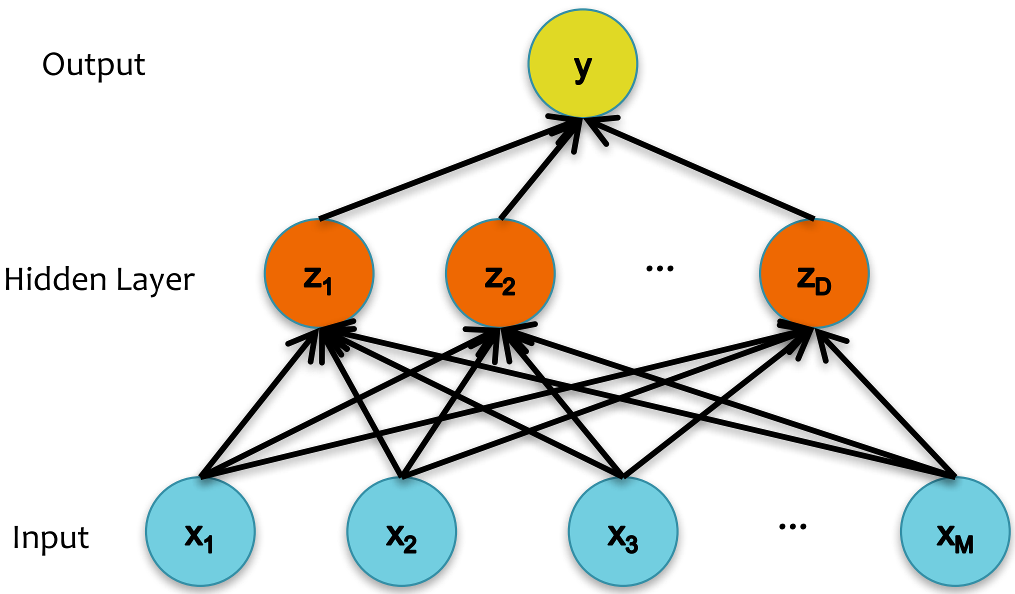
Neural Network with sigmoid activation functions





Activation Functions

Neural Network with arbitrary nonlinear activation functions



(F) **Loss**
$J = \frac{1}{2}(y - y^*)^2$

(E) **Output (nonlinear)**
$y = \sigma(b)$

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

(C) **Hidden (nonlinear)**
$z_j = \sigma(a_j), \ \forall j$

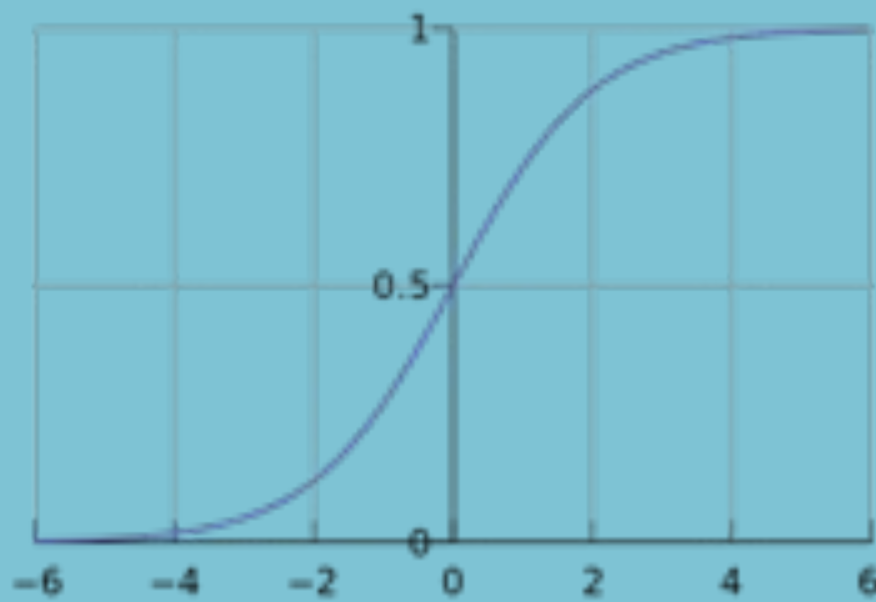
(B) **Hidden (linear)**
$a_j = \sum_{i=0}^{M} \alpha_{ji} x_i, \ \forall j$

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

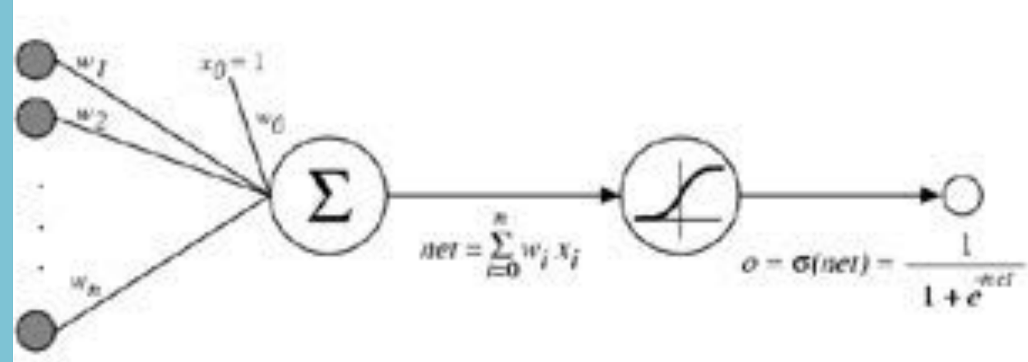
Activation Functions

Sigmoid / Logistic Function

$$\text{logistic}(u) \equiv \frac{1}{1+e^{-u}}$$

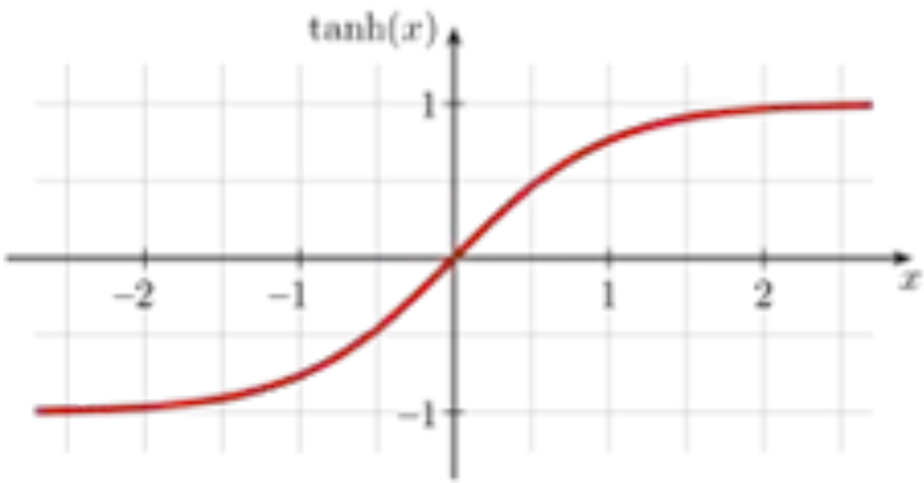


So far, we've assumed that the activation function (nonlinearity) is always the sigmoid function…



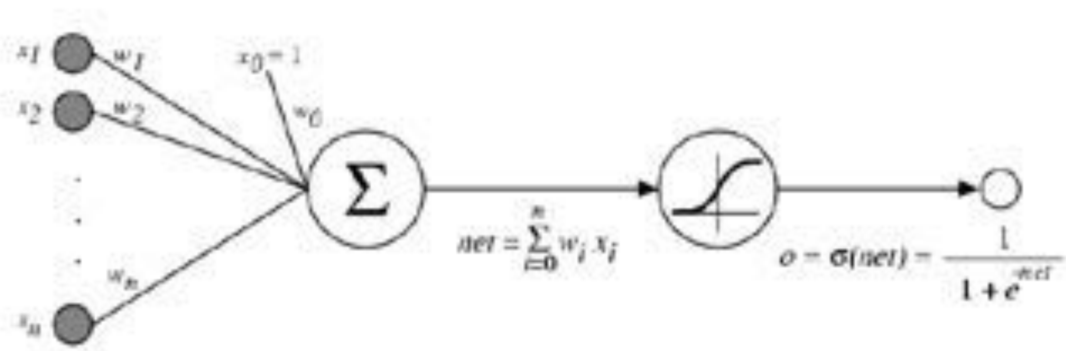
Activation Functions

- A new change: modifying the nonlinearity
  - The logistic is not widely used in modern ANNs



Alternate 1:
tanh

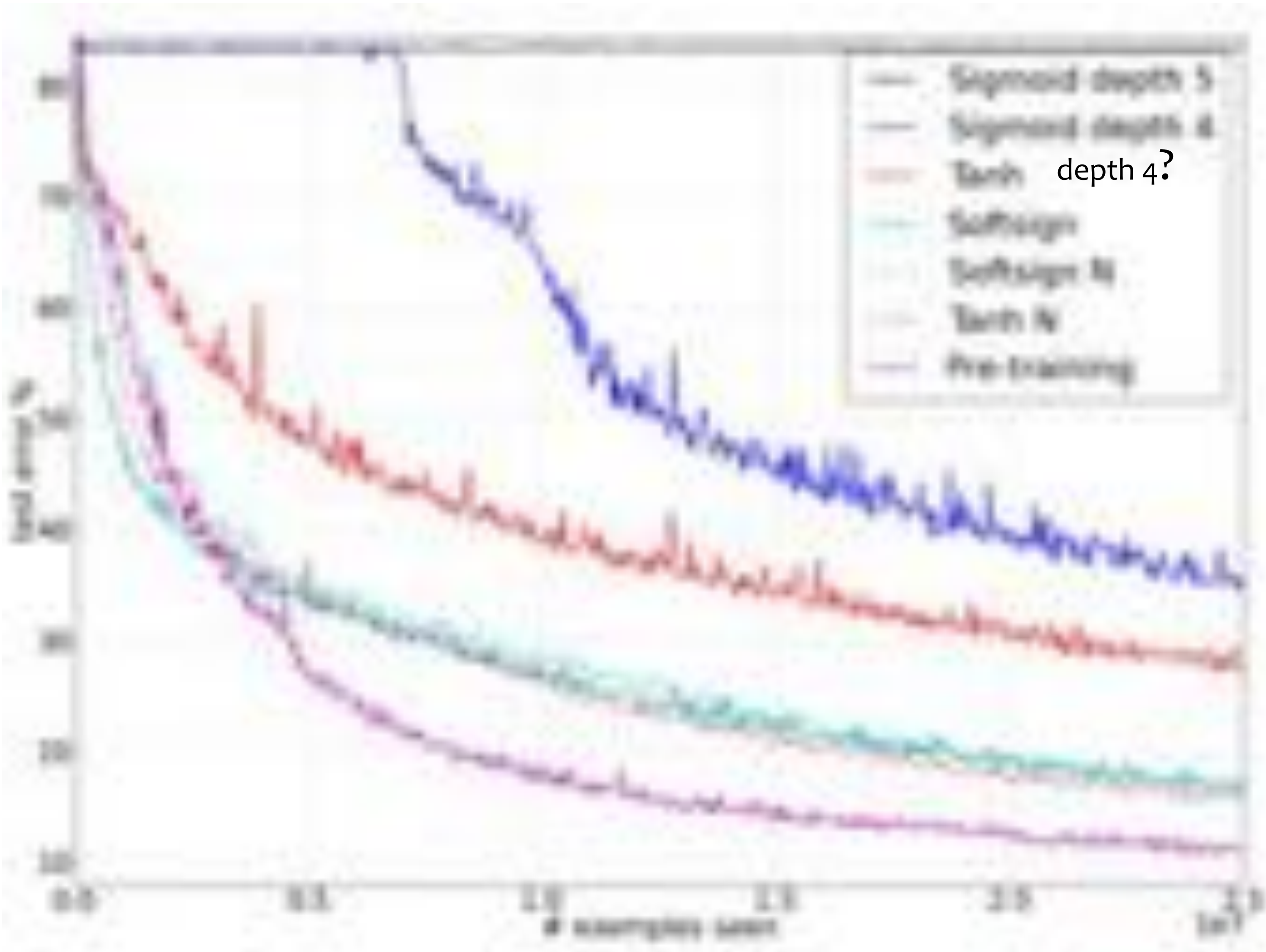
Like logistic function but shifted to range [-1, +1]



Slide from William Cohen

Understanding the difficulty of training deep feedforward neural networks

AI Stats 2010

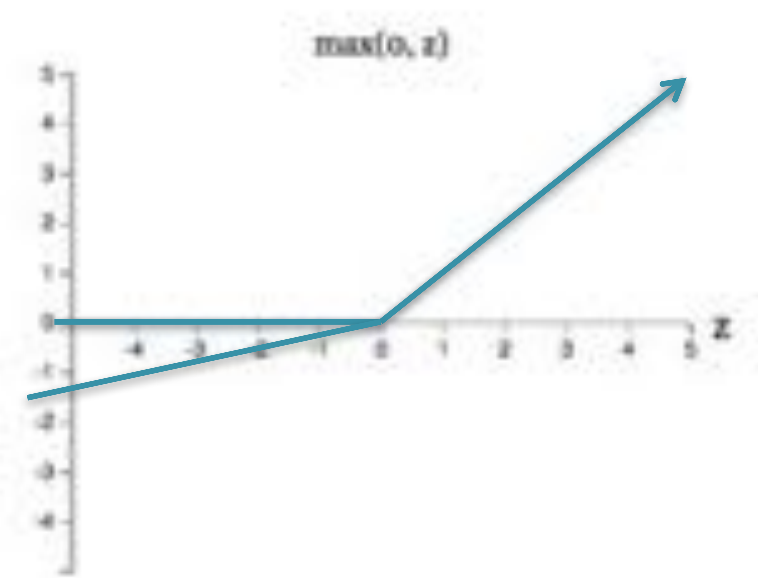


sigmoid
vs.
tanh

Figure from Glorot & Bentio (2010)

Activation Functions

- A new change: modifying the nonlinearity
  - reLU often used in vision tasks

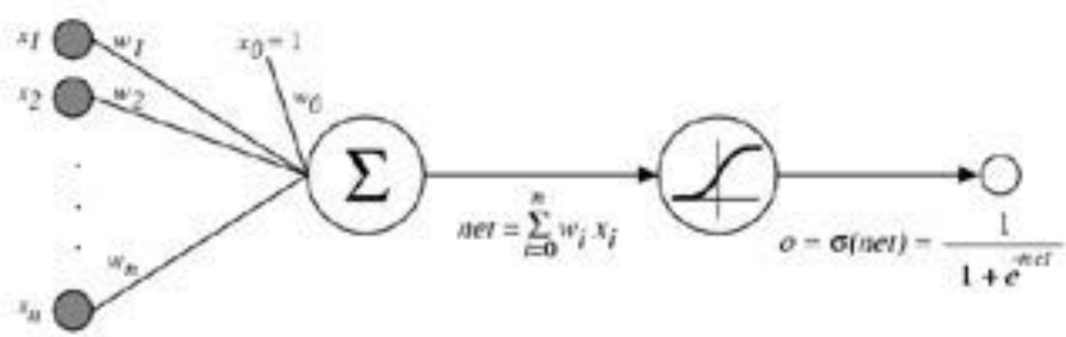


$$\max(0, w \cdot x + b).$$

Alternate 2: rectified linear unit

Linear with a cutoff at zero

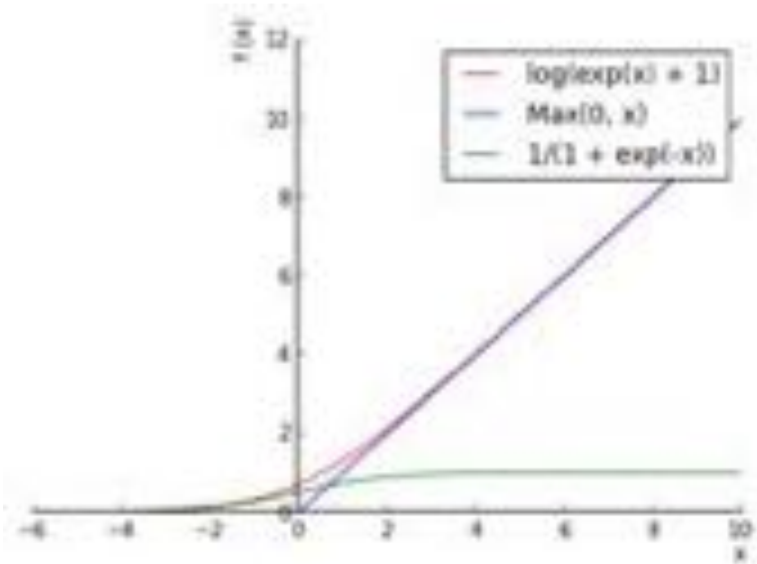
(Implementation: clip the gradient when you pass zero)



Slide from William Cohen

Activation Functions

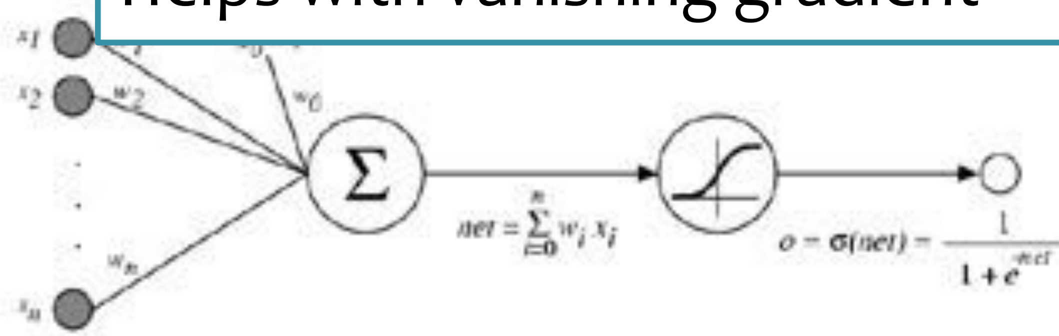
- A new change: modifying the nonlinearity
  - reLU often used in vision tasks



Alternate 2: rectified linear unit

Soft version: log(exp(x)+1)

Doesn't saturate (at one end)
Sparsifies outputs
Helps with vanishing gradient



Slide from William Cohen

Objective Functions for NNs

1. Quadratic Loss:
   – the same objective as Linear Regression
   – i.e. mean squared error
2. Cross-Entropy:
   – the same objective as Logistic Regression
   – i.e. negative log likelihood
   – This requires probabilities, so we add an additional "softmax" layer at the end of our network

	Forward	Backward
Quadratic	$J = \frac{1}{2}(y - y^*)^2$	$\frac{dJ}{dy} = y - y^*$
Cross Entropy	$J = y^* \log(y) + (1 - y^*) \log(1 - y)$	$\frac{dJ}{dy} = y^* \frac{1}{y} + (1 - y^*) \frac{1}{y - 1}$

Objective Functions for NNs

Cross-entropy vs. Quadratic loss

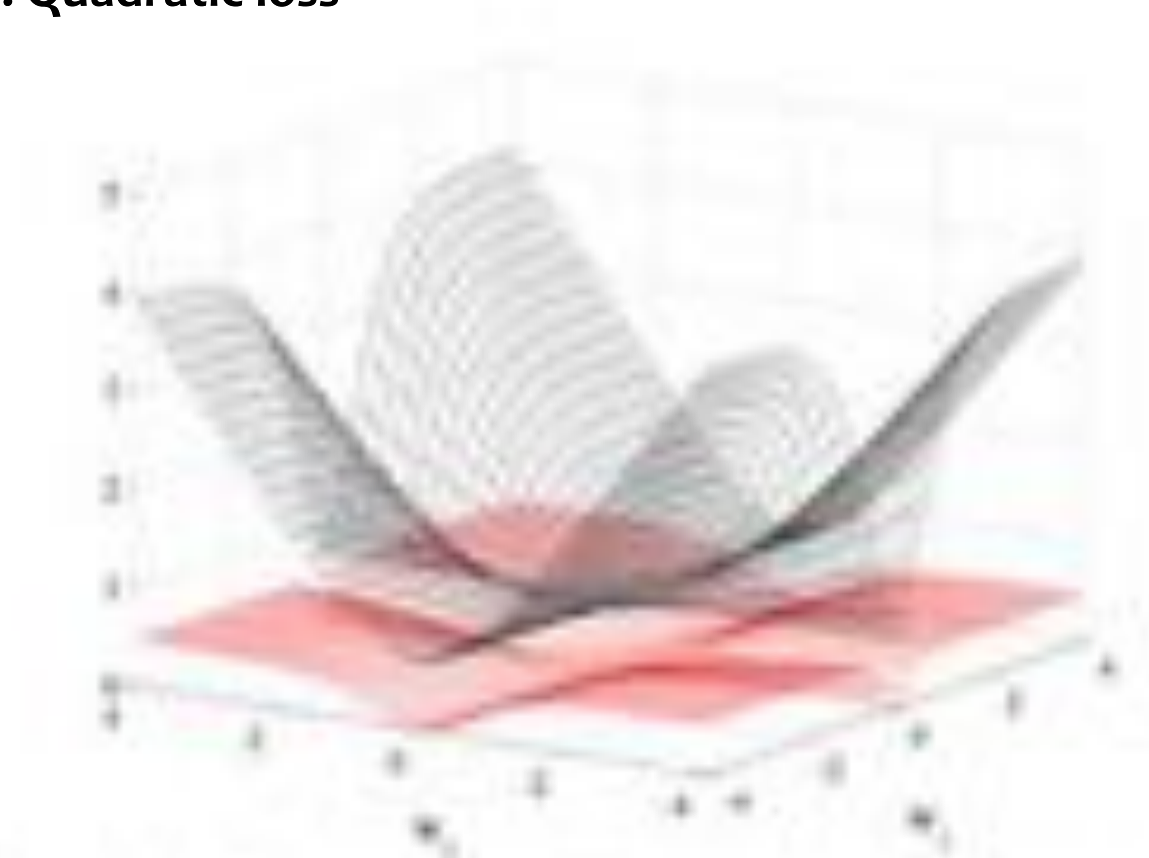
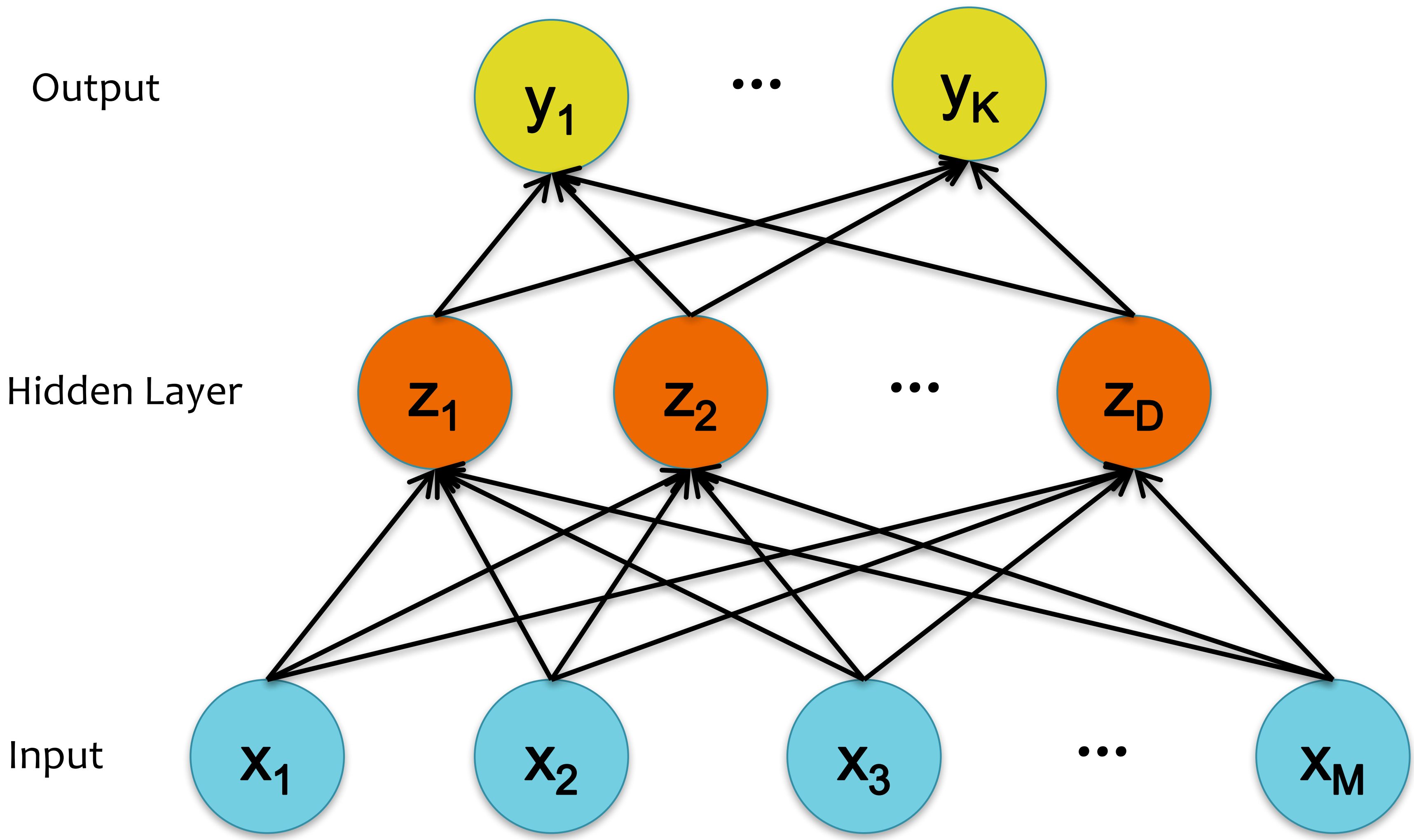


Figure 5: Cross entropy (black, surface on top) and quadratic (red, bottom surface) cost as a function of two weights (one at each layer) of a network with two layers, W_1 respectively on the first layer and W_2 on the second, output layer.

Figure from Glorot & Bentio (2010)

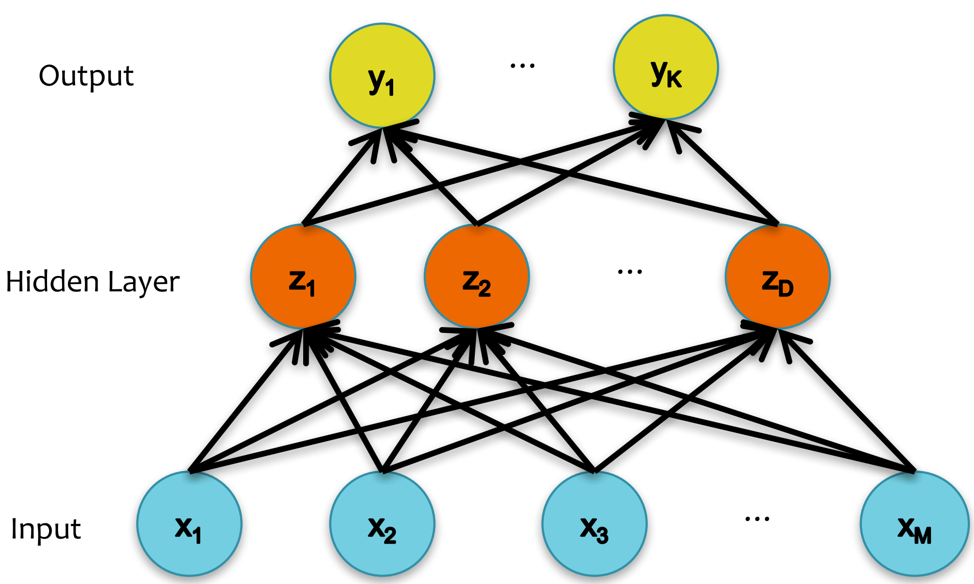
Multi-Class Output



Multi-Class Output

Softmax:

$$y_k = \frac{\exp(b_k)}{\sum_{l=1}^{K} \exp(b_l)}$$



(F) Loss
$J = \sum_{k=1}^{K} y_k^* \log(y_k)$

(E) Output (softmax)
$y_k = \frac{\exp(b_k)}{\sum_{l=1}^{K} \exp(b_l)}$

(D) Output (linear)
$b_k = \sum_{j=0}^{D} \beta_{kj} z_j \ \forall k$

(C) Hidden (nonlinear)
$z_j = \sigma(a_j), \ \forall j$

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

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

Neural Networks Objectives

You should be able to…

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