10-601 Introduction to Machine Learning

Machine Learning Department
School of Computer Science
Carnegie Mellon University

Neural Networks and Backpropagation

Neural Net Readings:

Murphy --
Bishop 5
HTF 11
Mitchell 4

Matt Gormley
Lecture 20
April 3, 2017

Reminders

- Homework 6: Unsupervised Learning
  - Release: Wed, Mar. 22
  - Due: Mon, Apr. 03 at 11:59pm
- Homework 5 (Part II): Peer Review
  - Release: Wed, Mar. 29
  - Due: Wed, Apr. 05 at 11:59pm
- Peer Tutoring

Expectation: You should spend at most 1 hour on your reviews

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

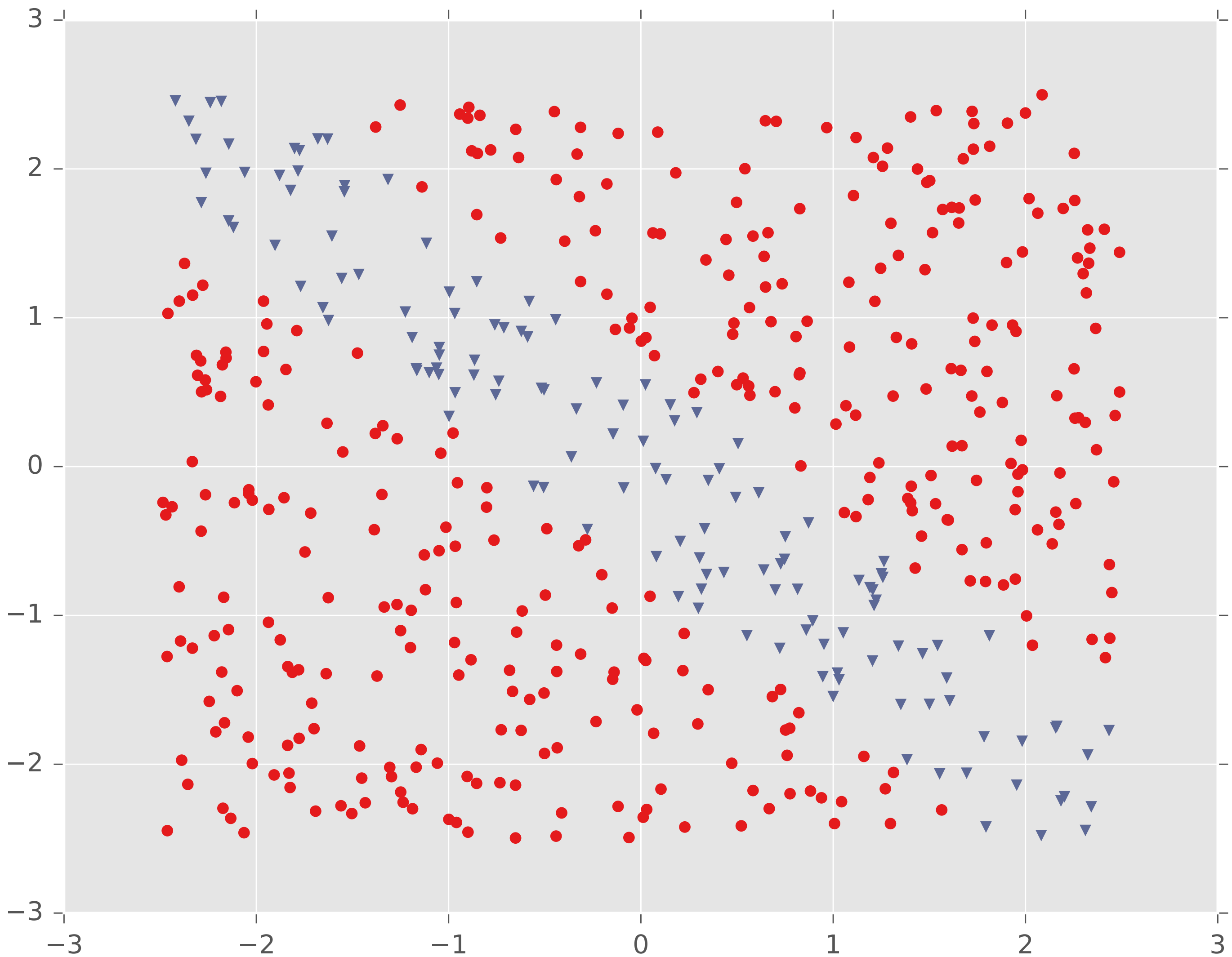
Last Lecture

- **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)

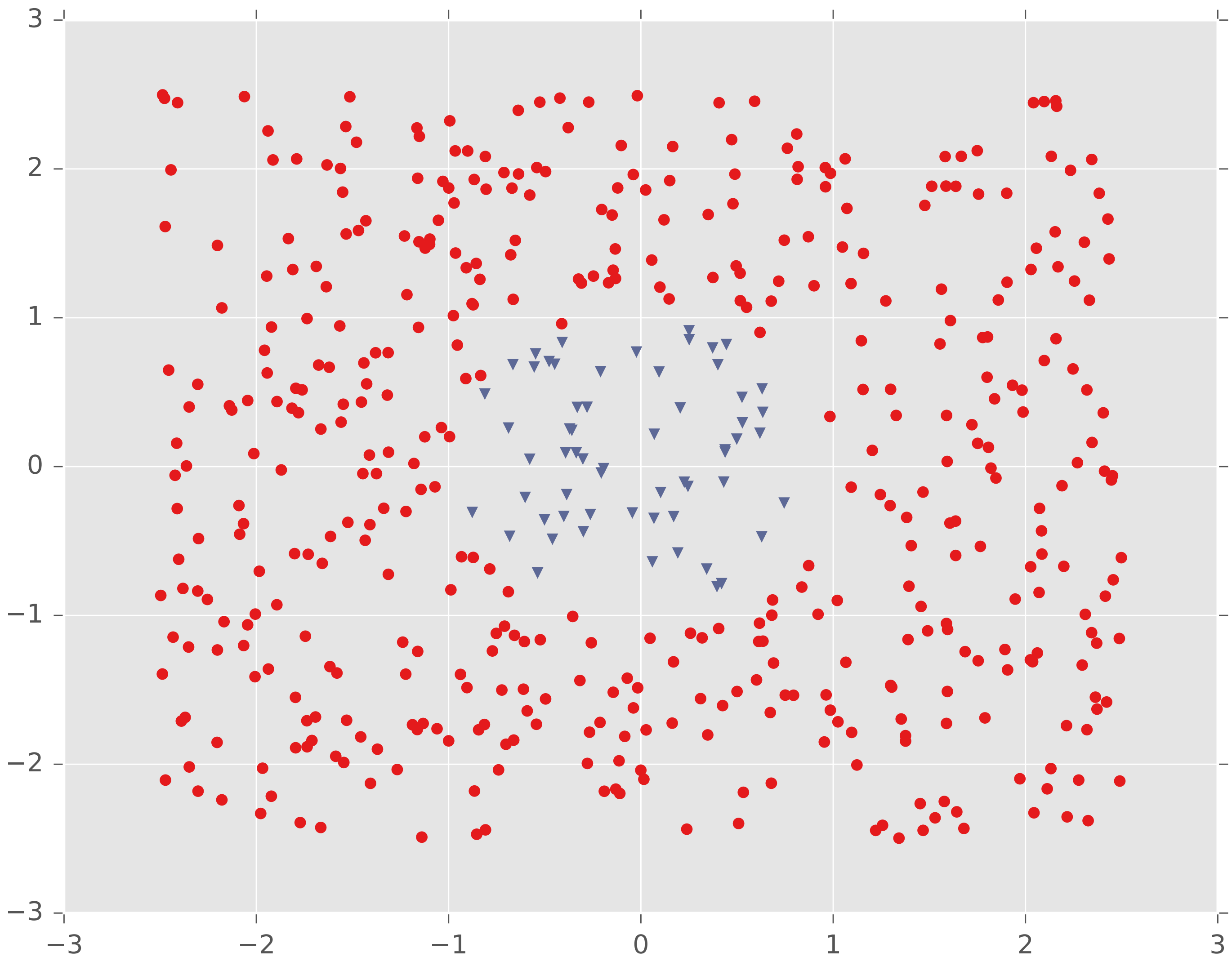
This Lecture

DECISION BOUNDARY EXAMPLES

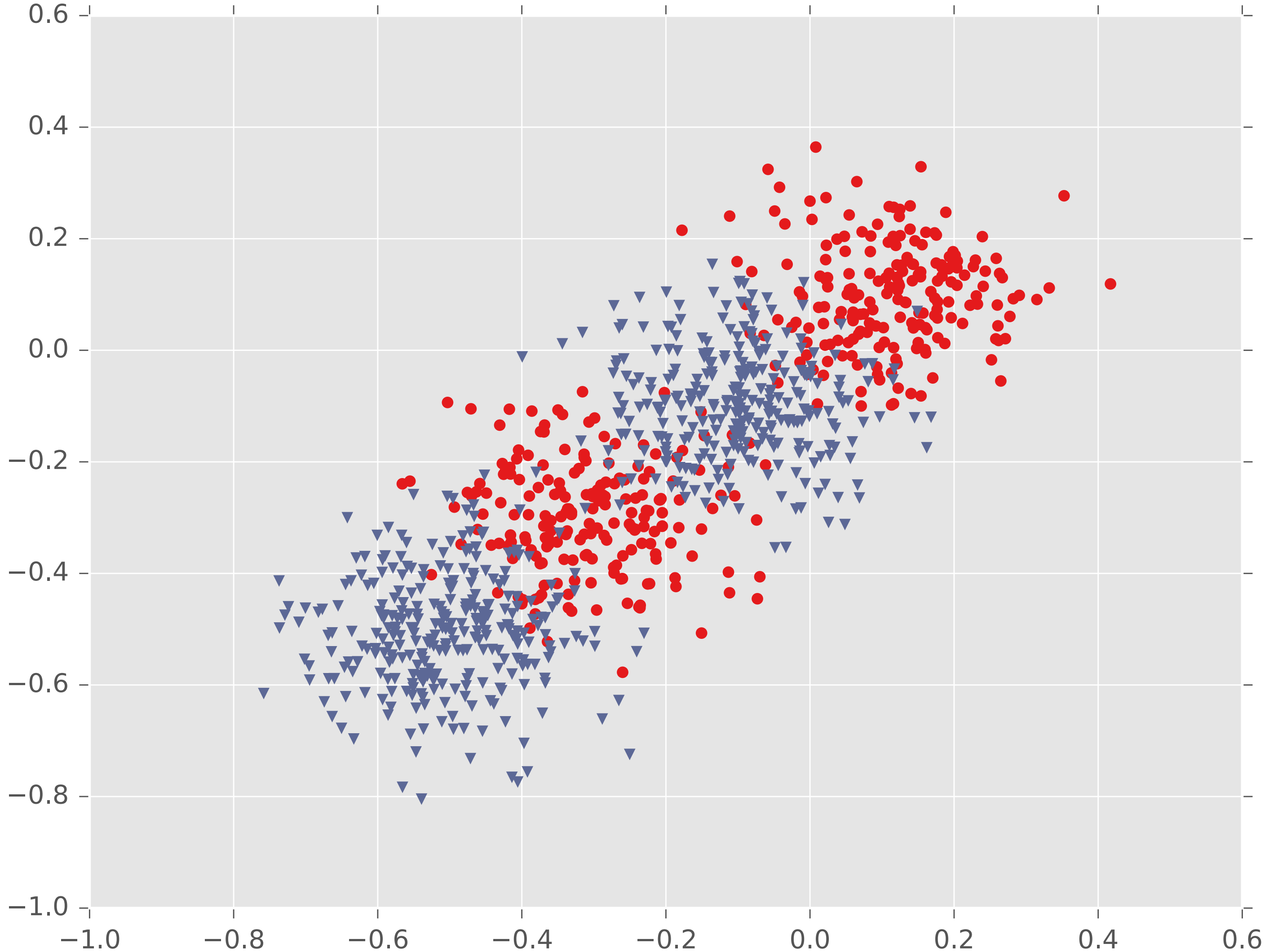
Example #1: Diagonal Band



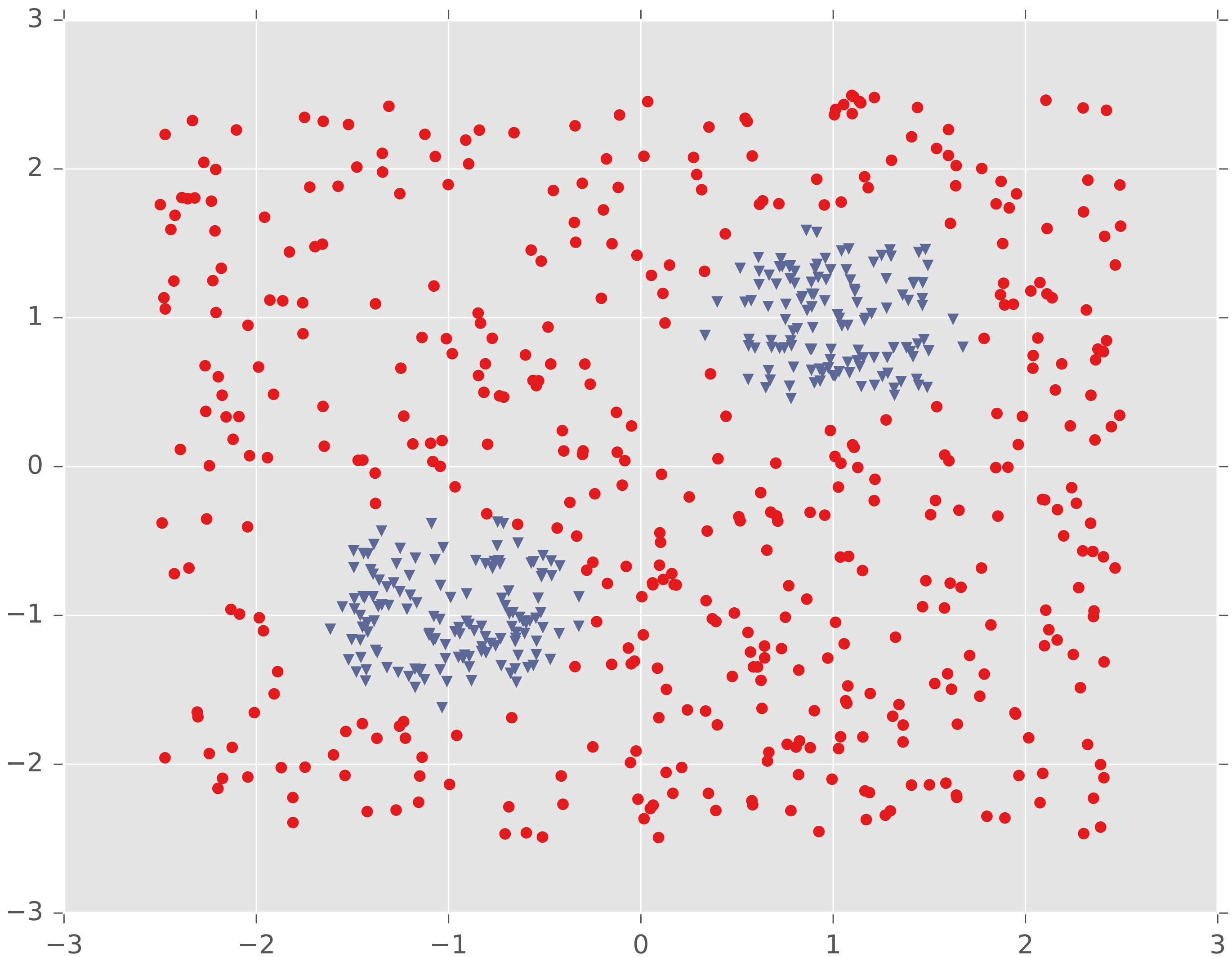
Example #2: One Pocket



Example #3: Four Gaussians



Example #4: Two Pockets



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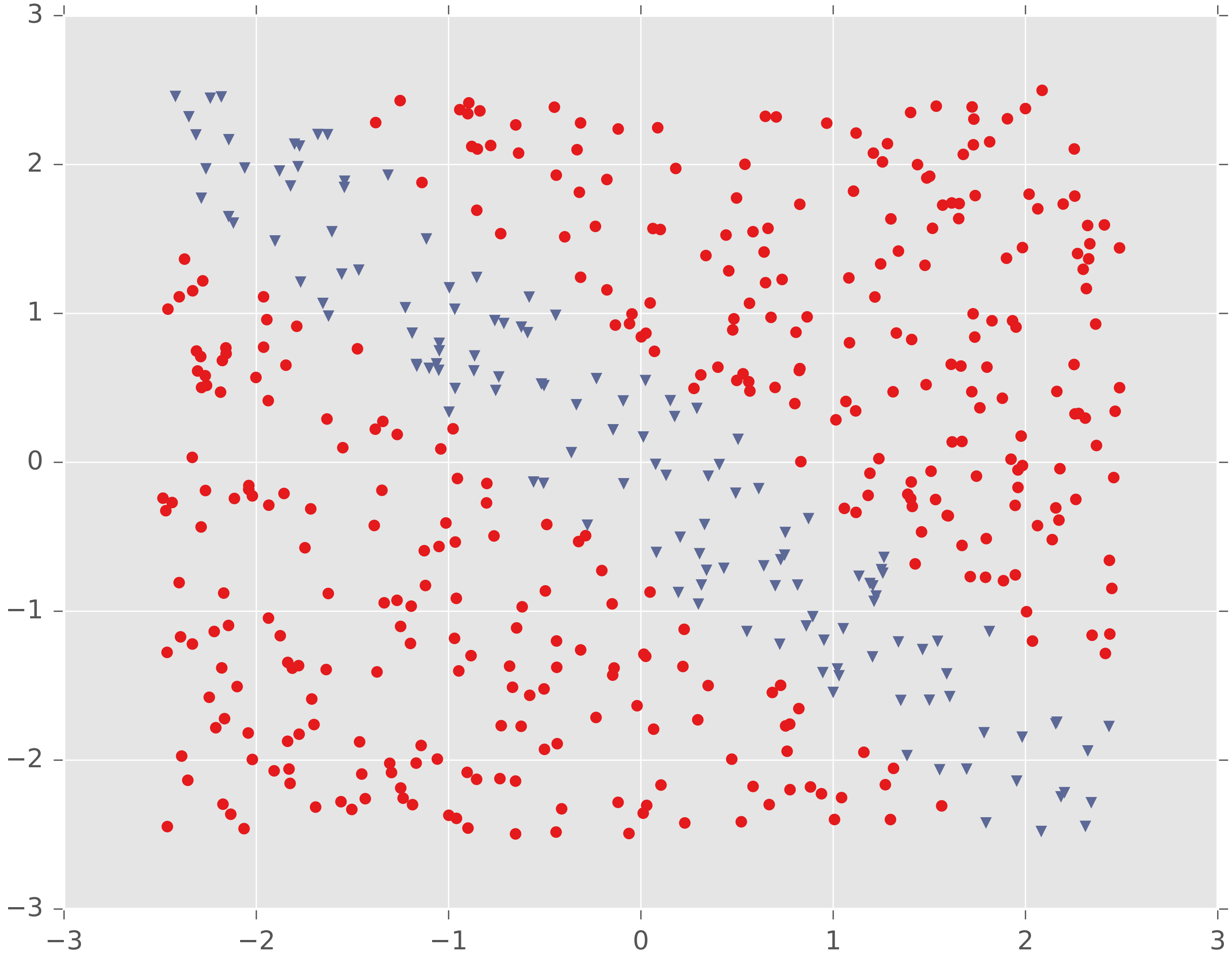

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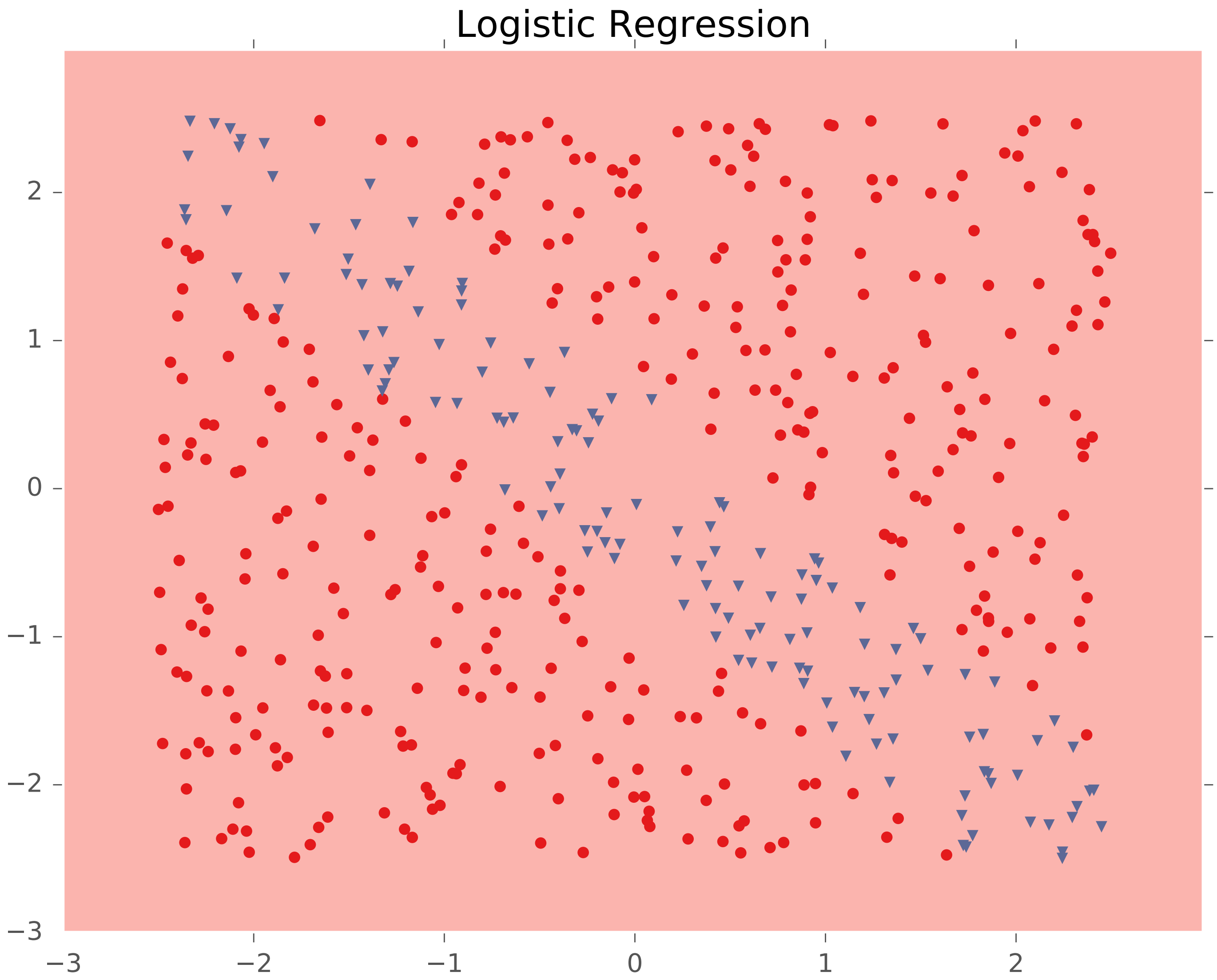

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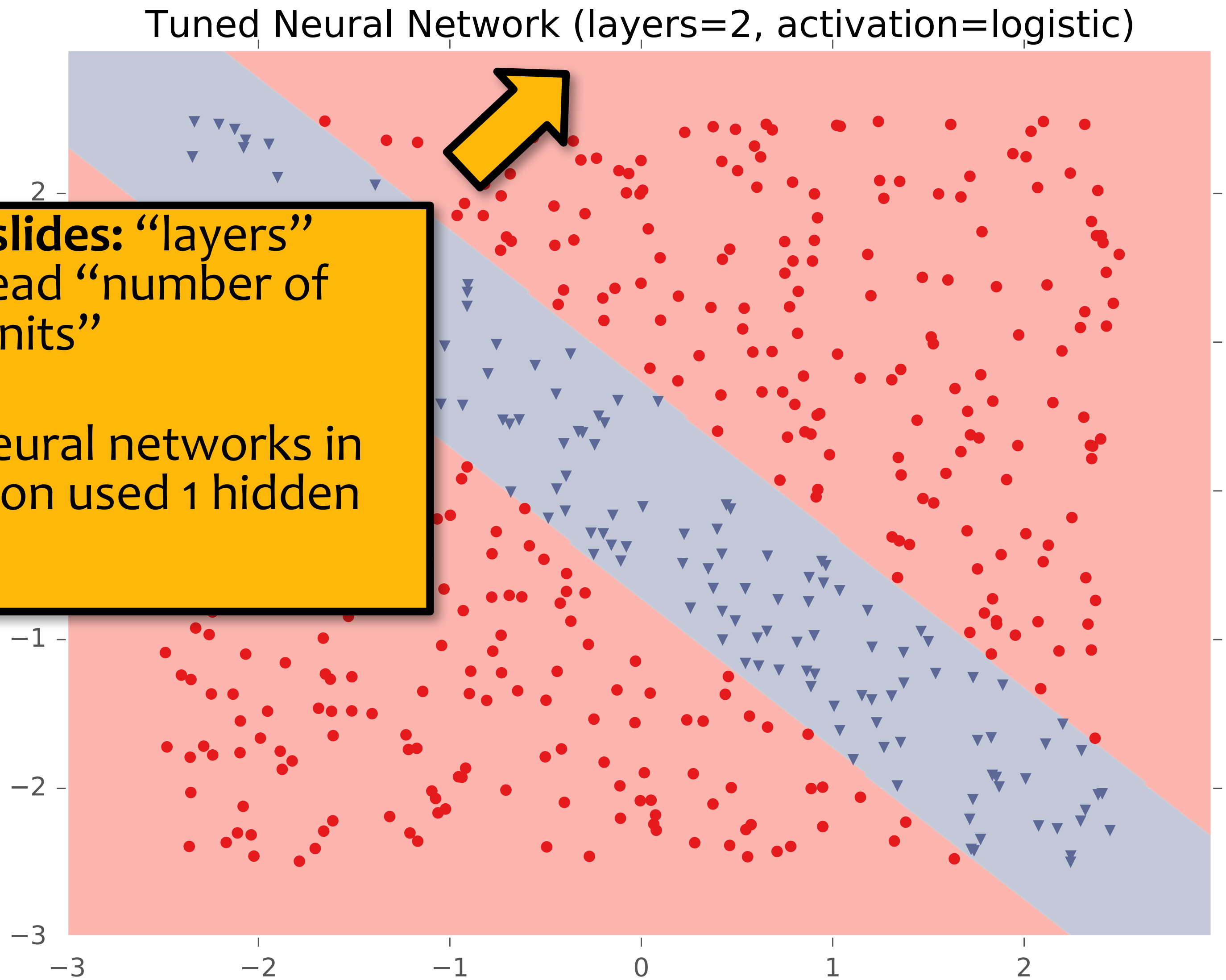

Error in slides: "layers" should read "number of hidden units"

All the neural networks in this section used 1 hidden layer.

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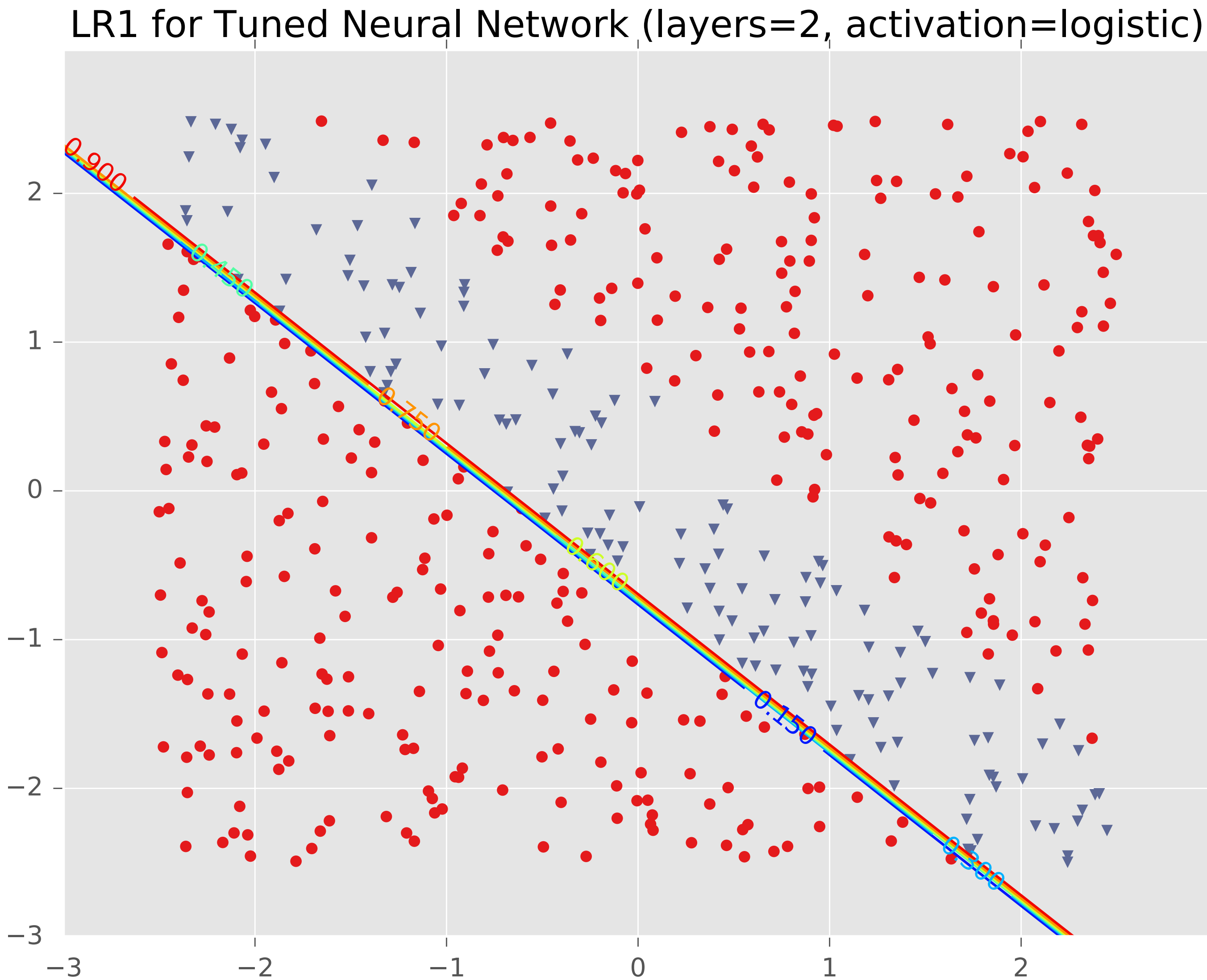

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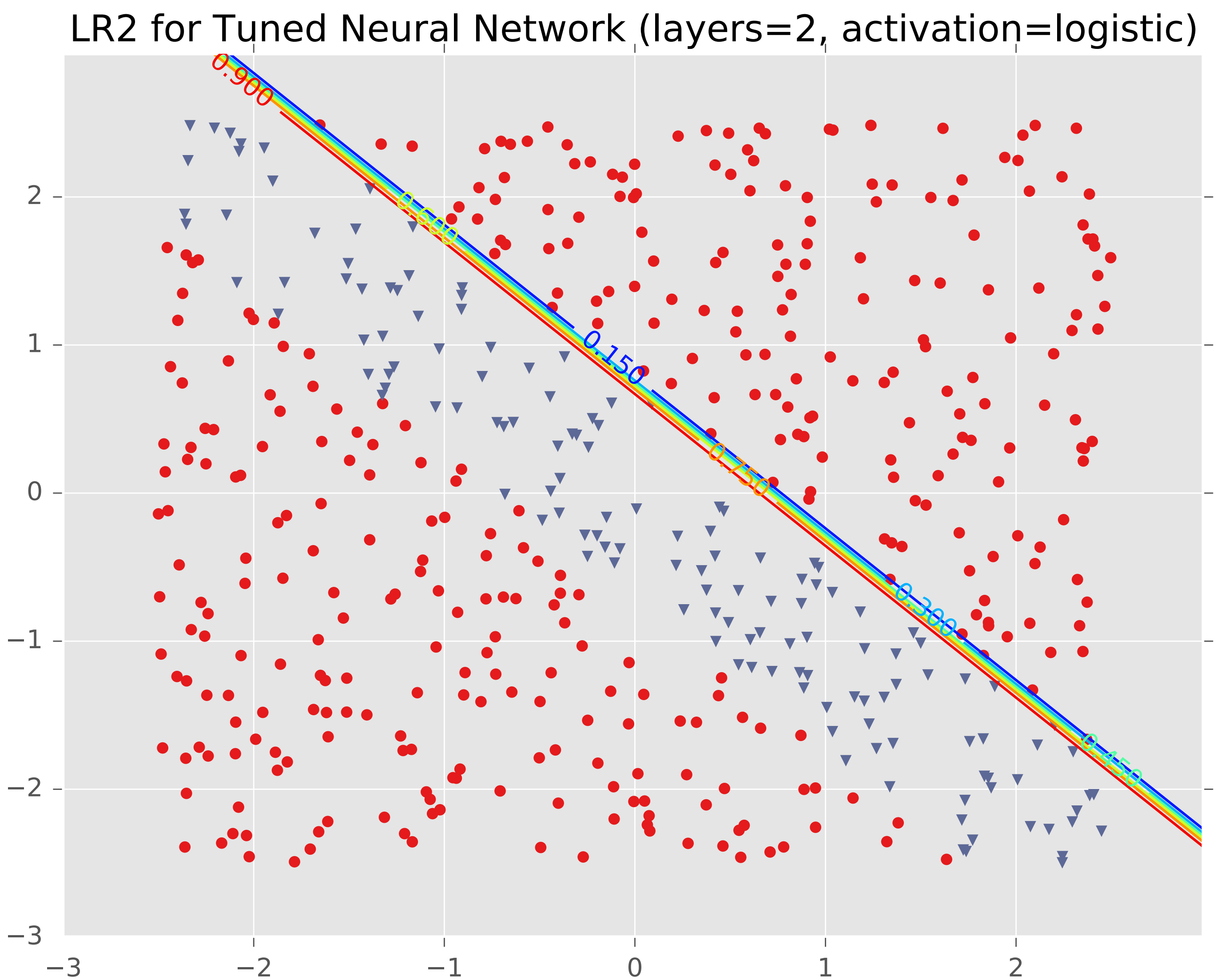

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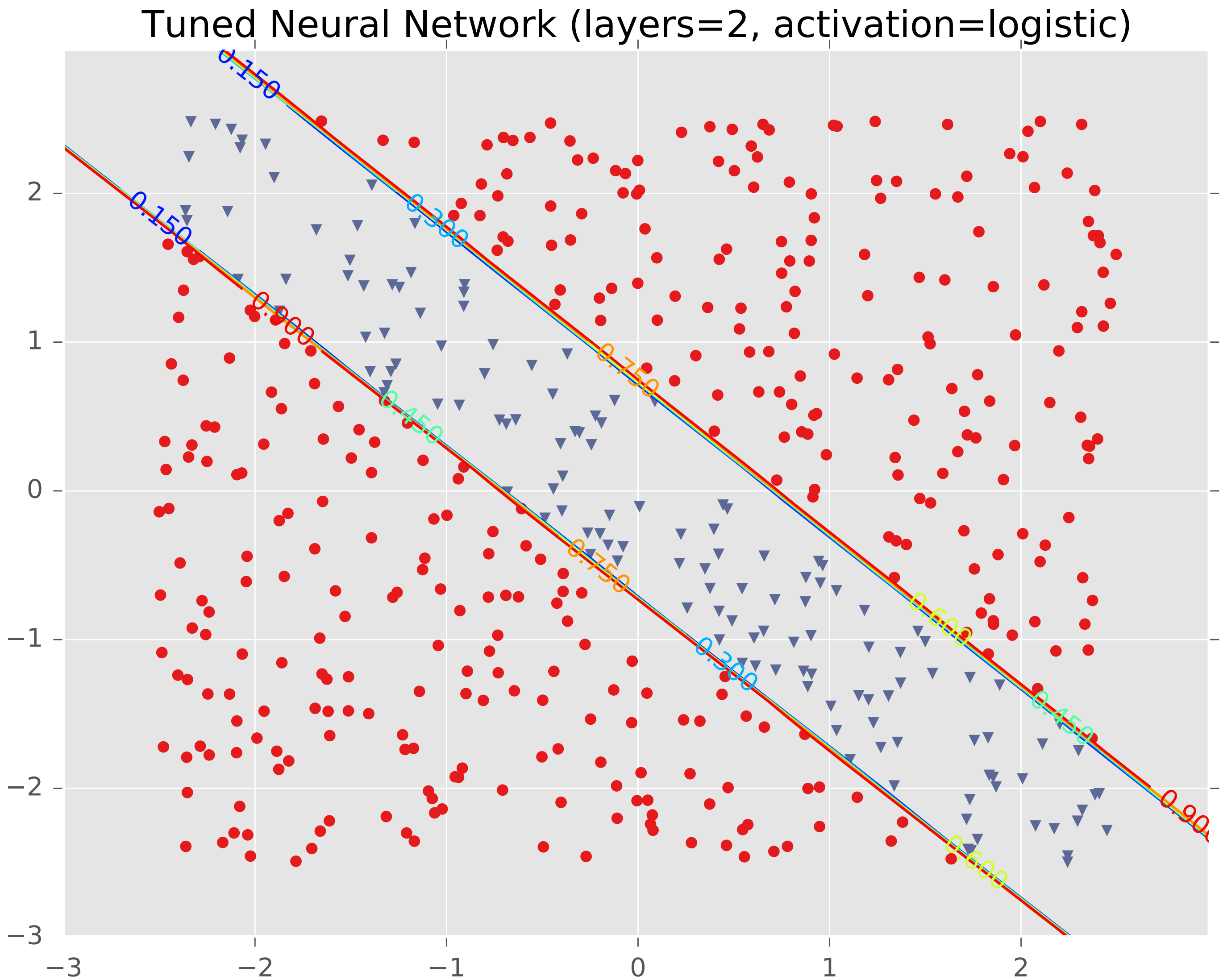

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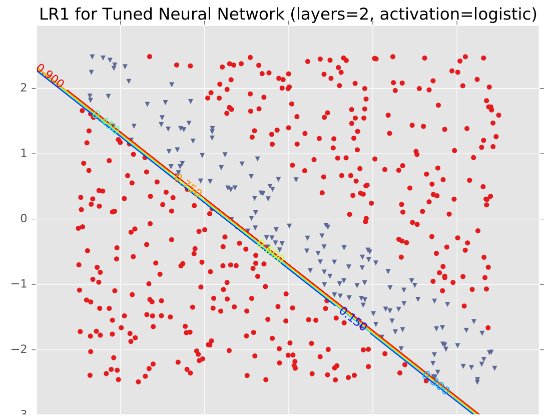

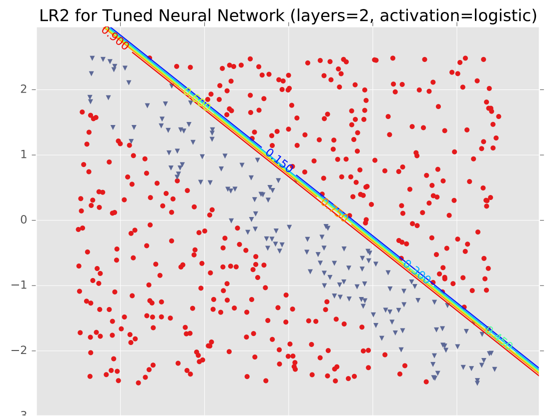

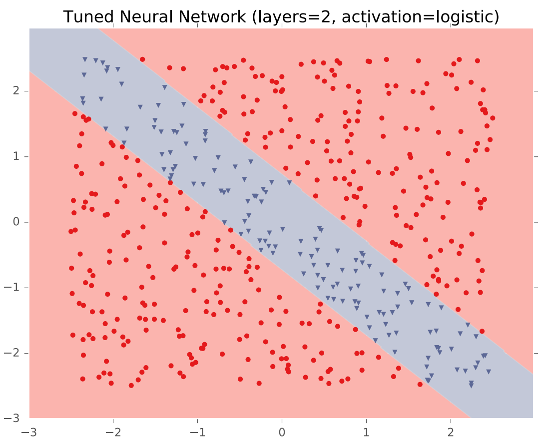

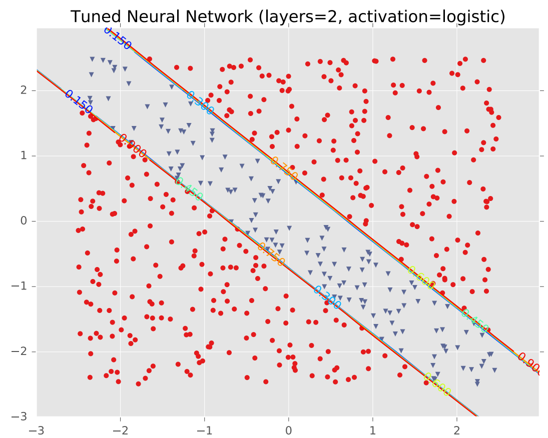

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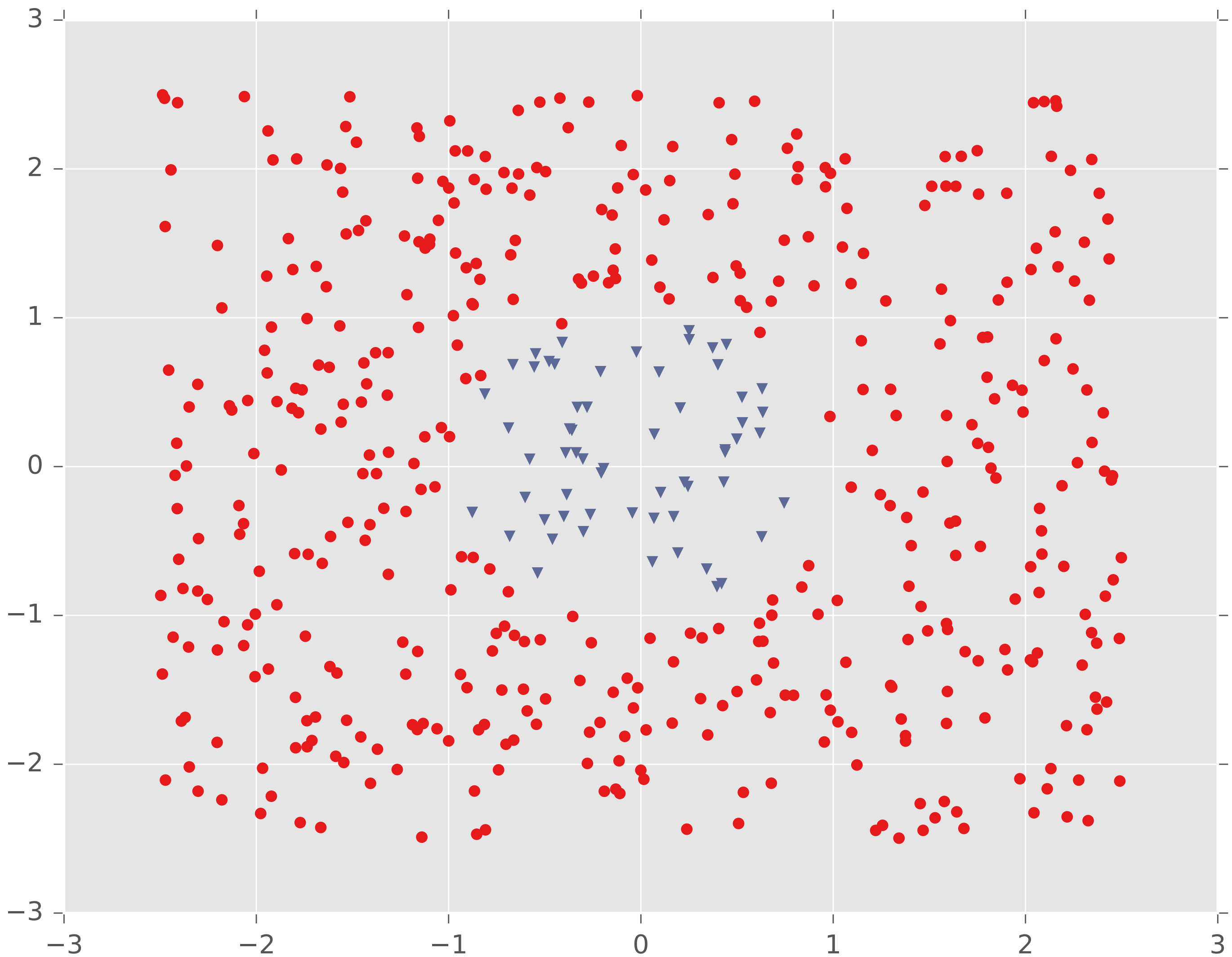

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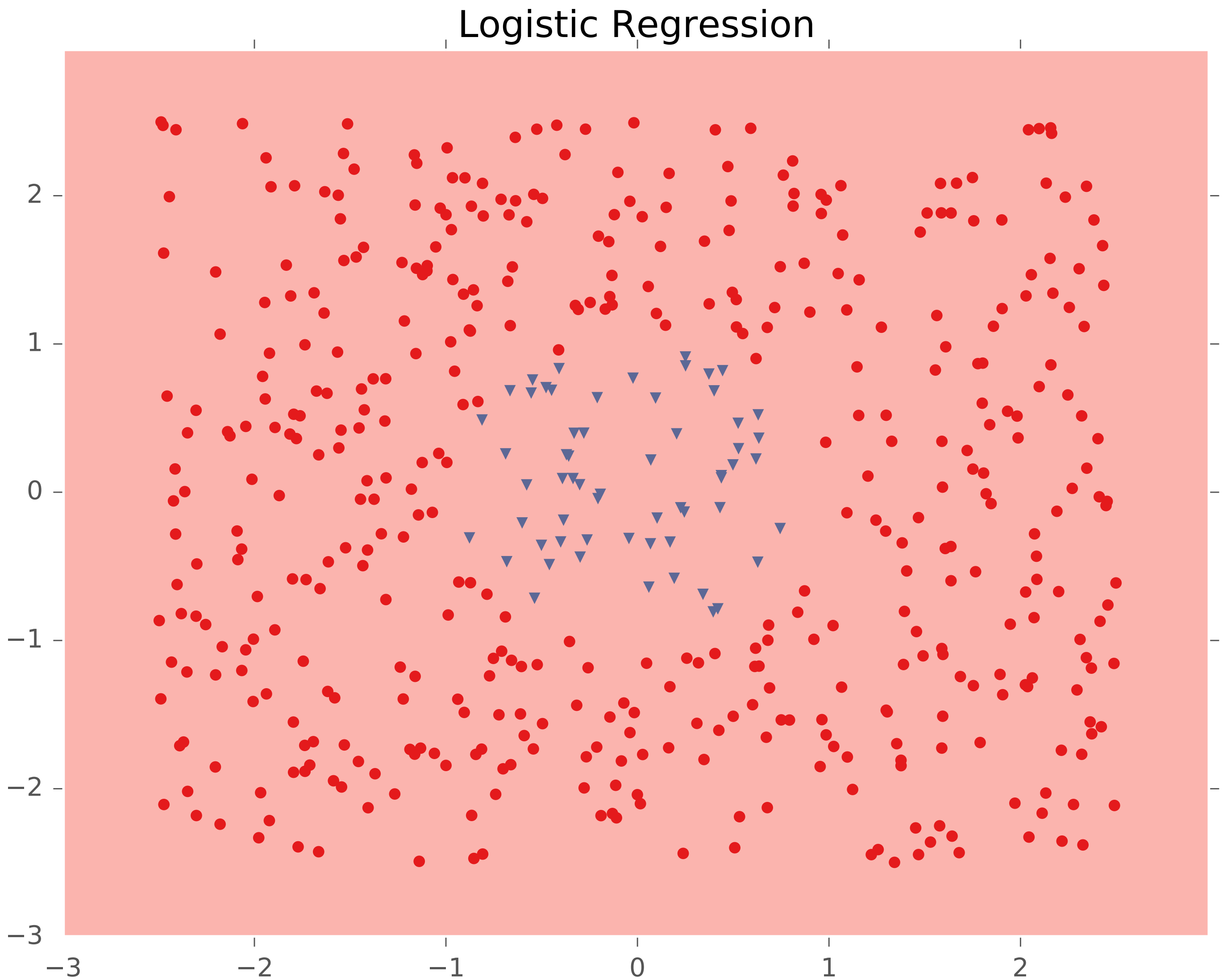

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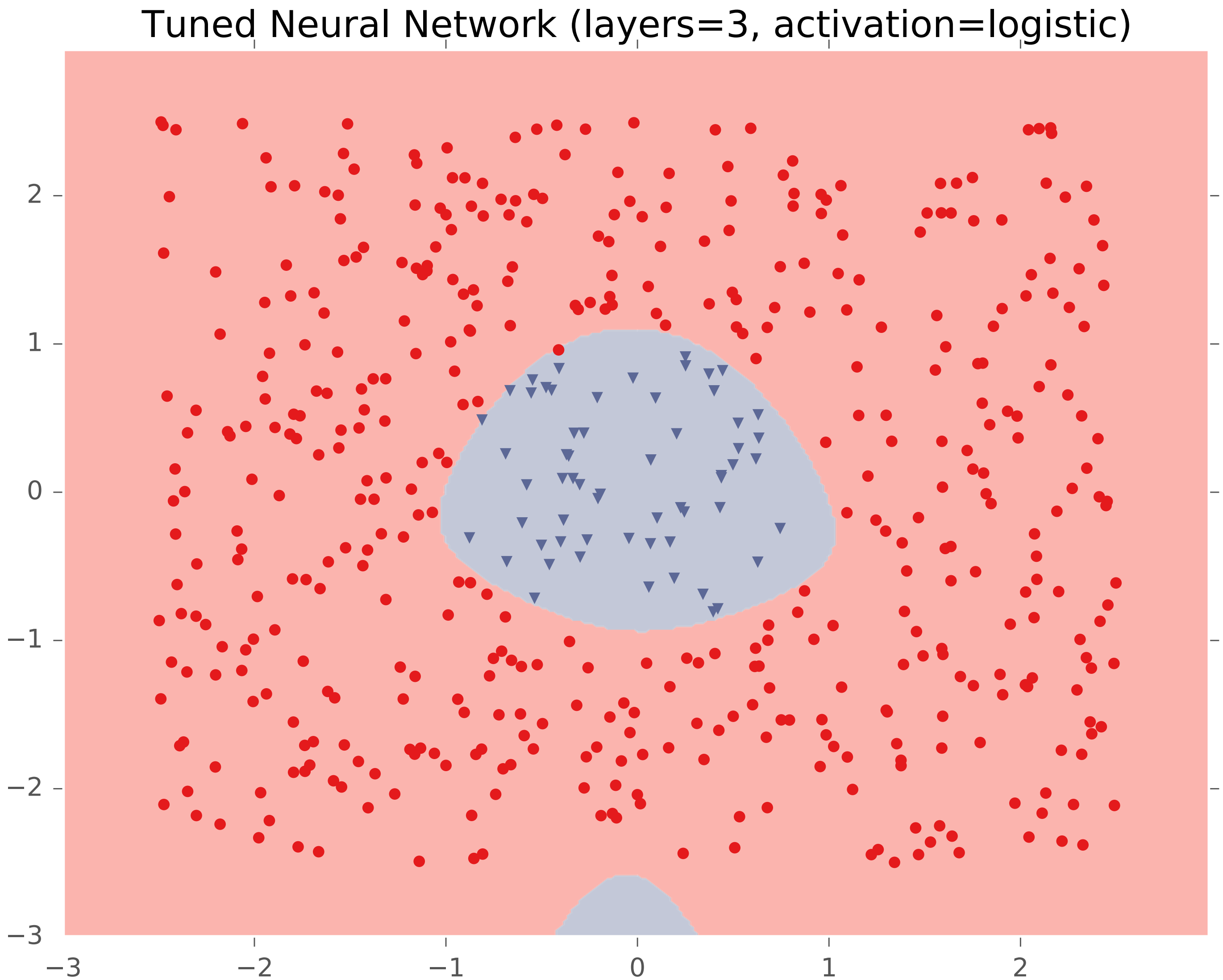

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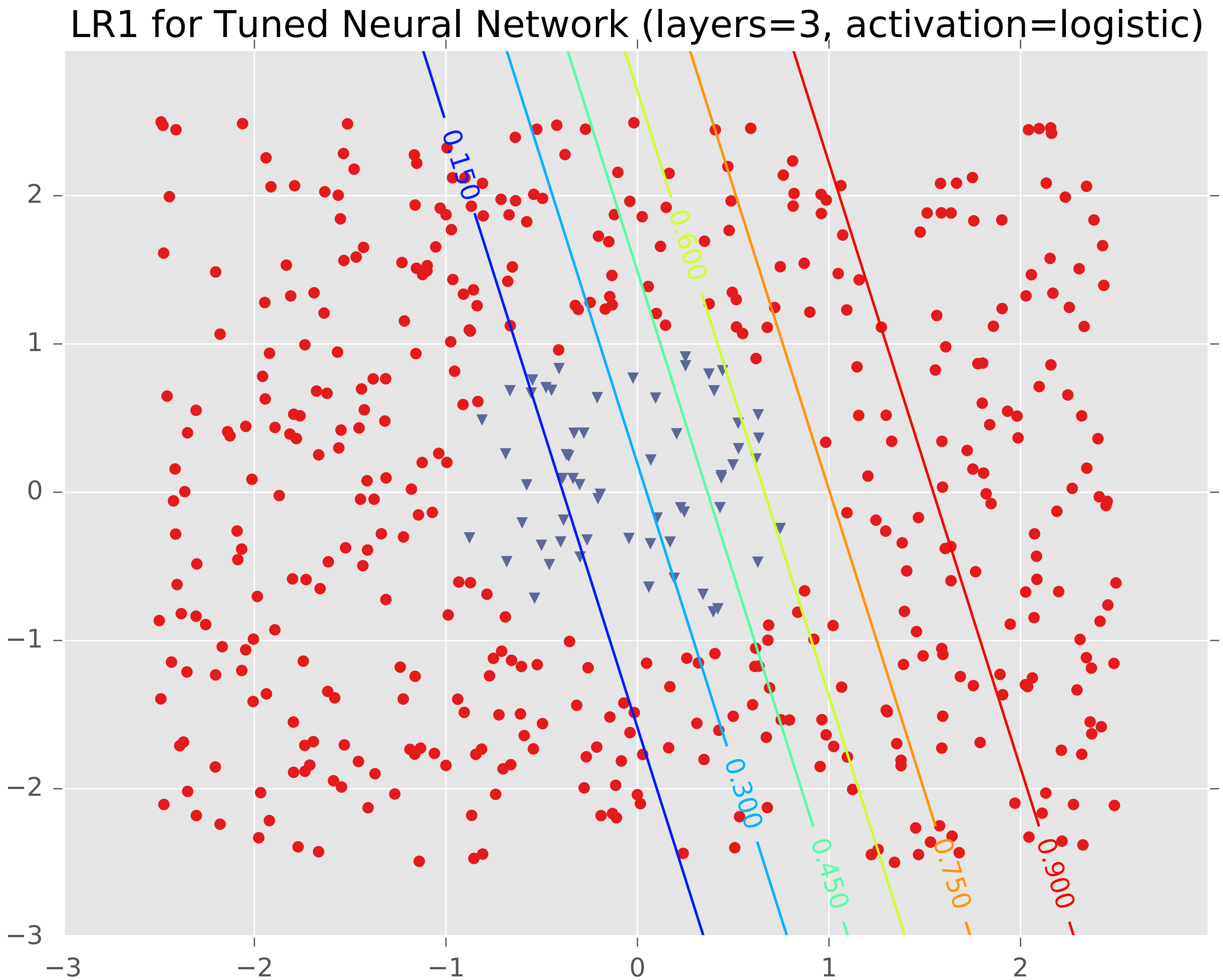

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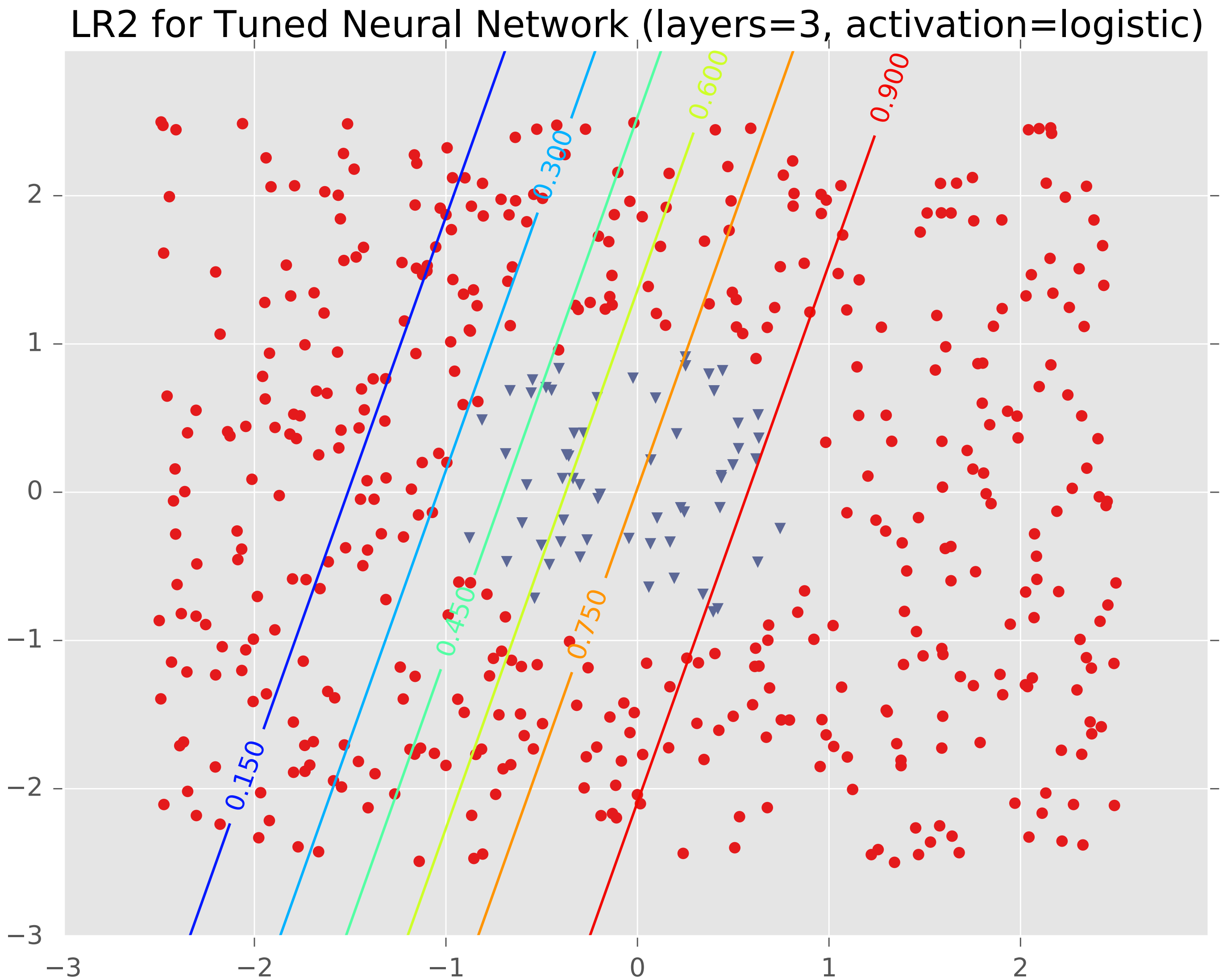

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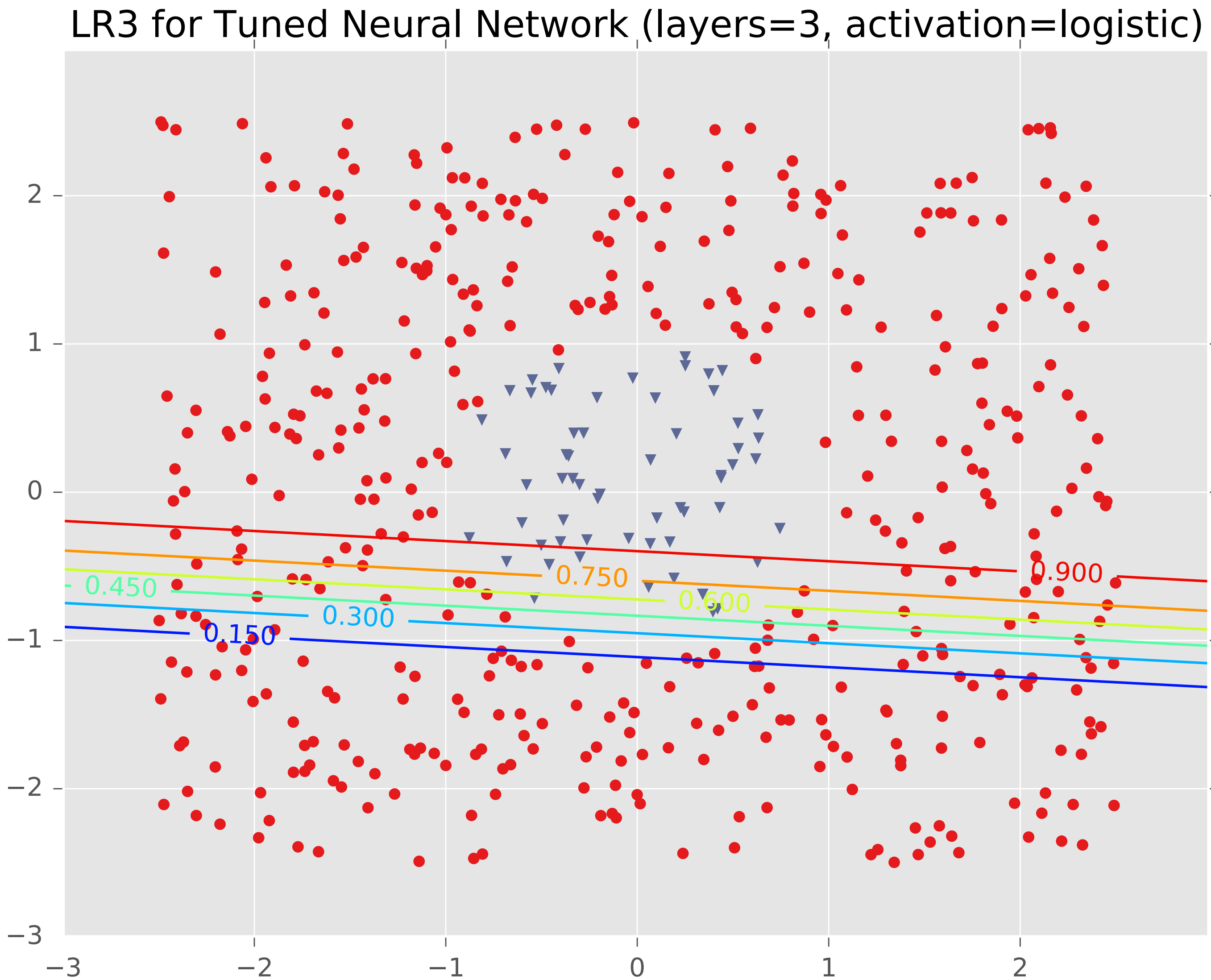

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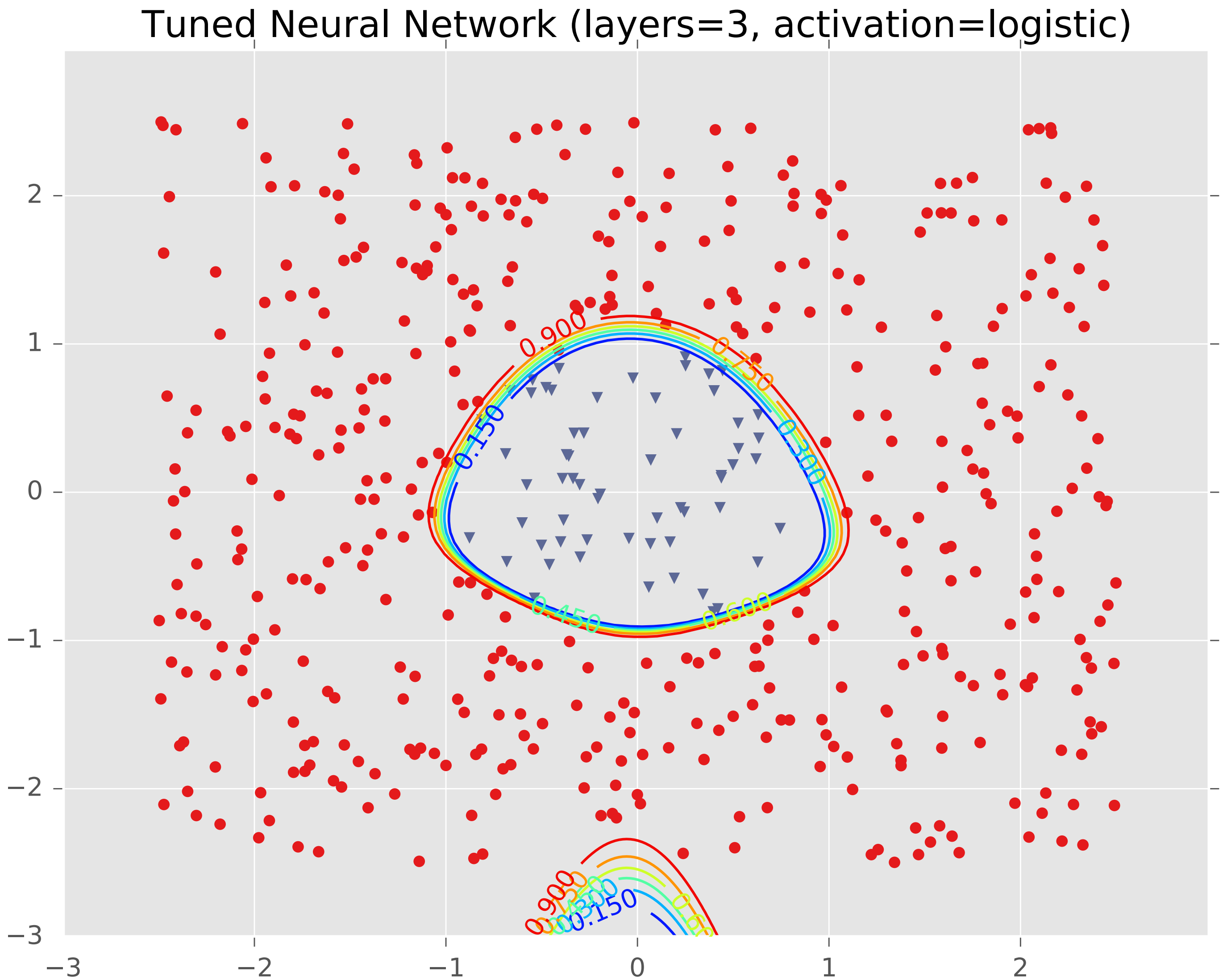

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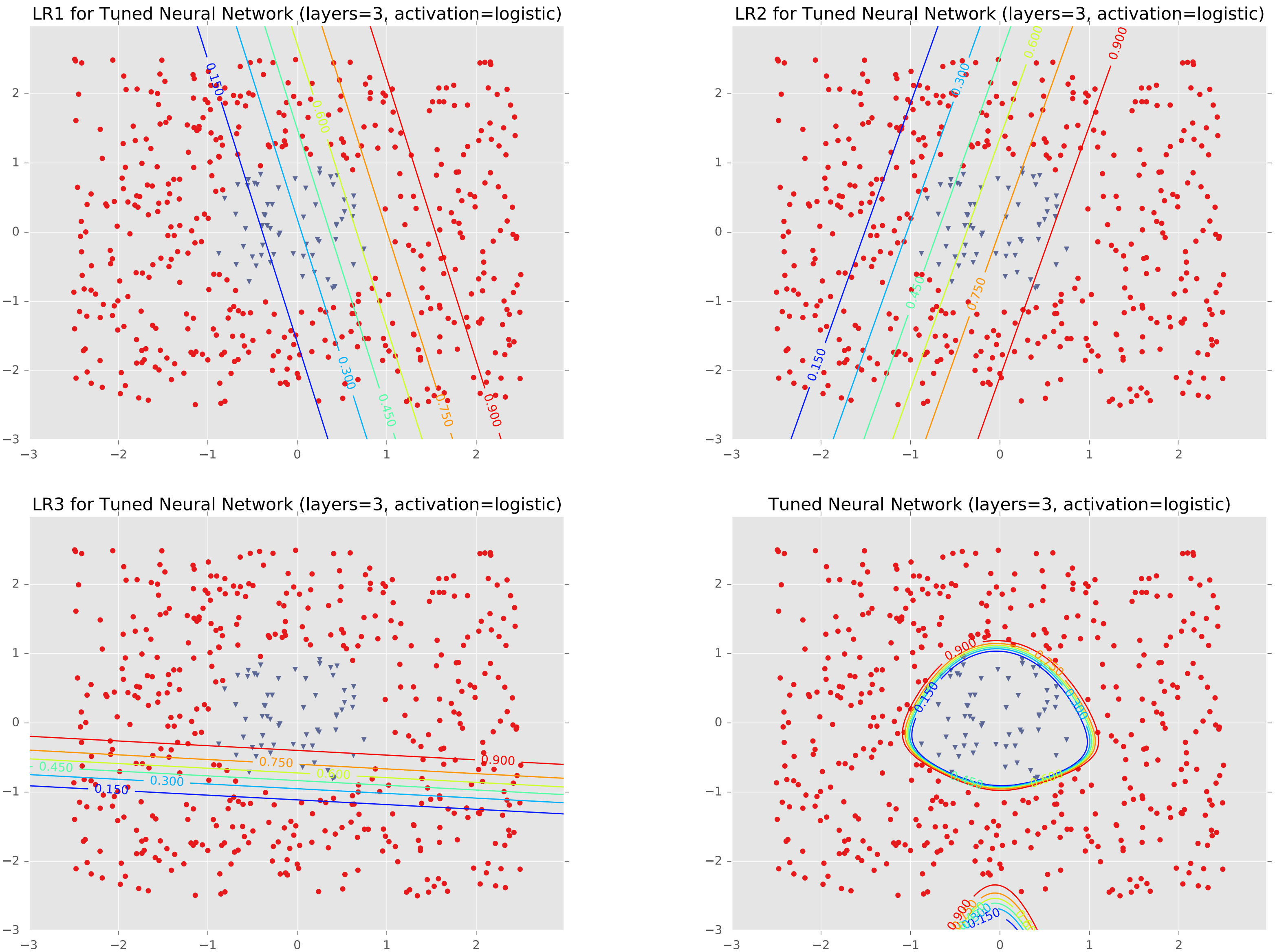

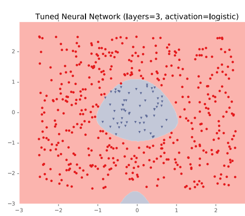

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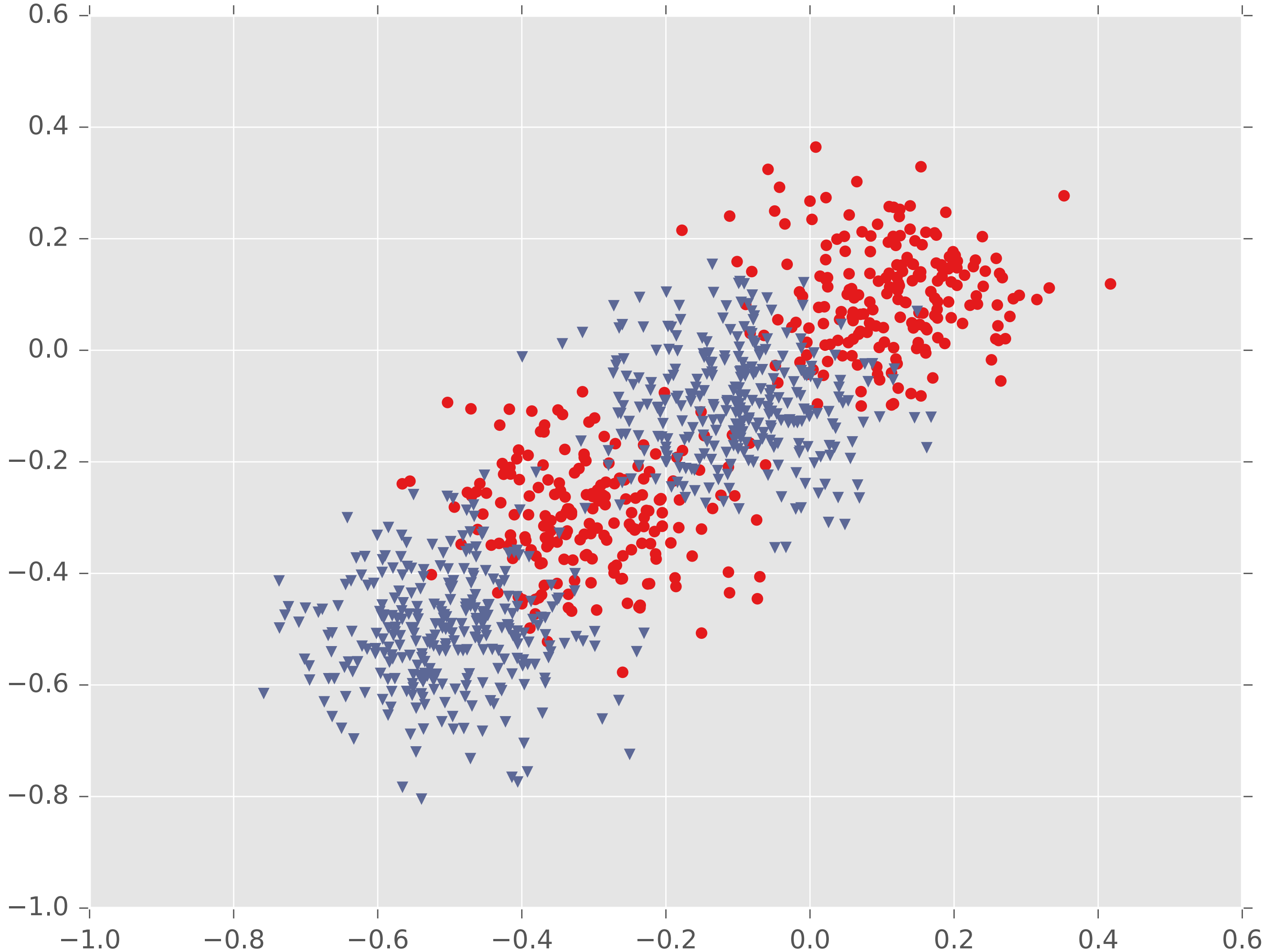

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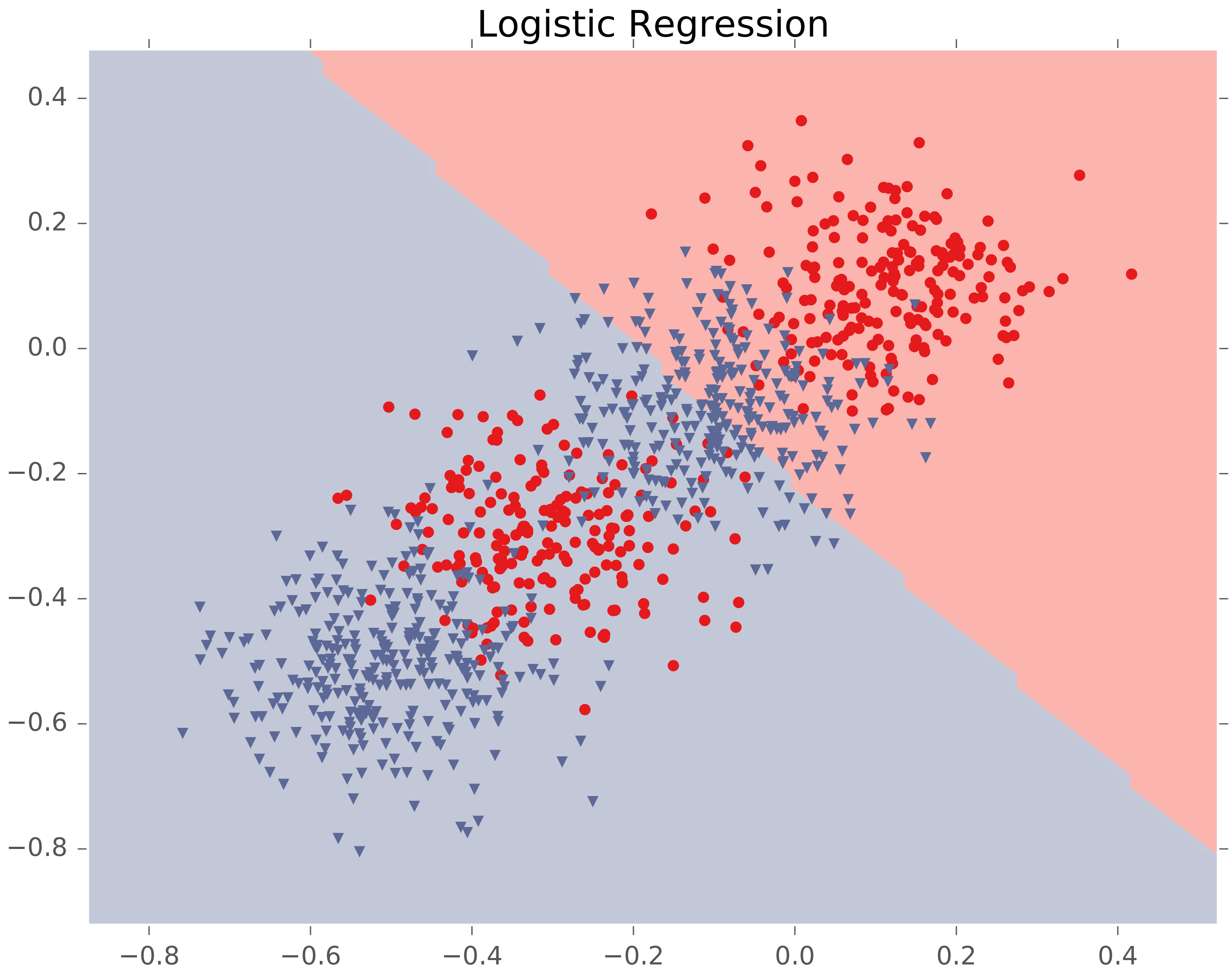

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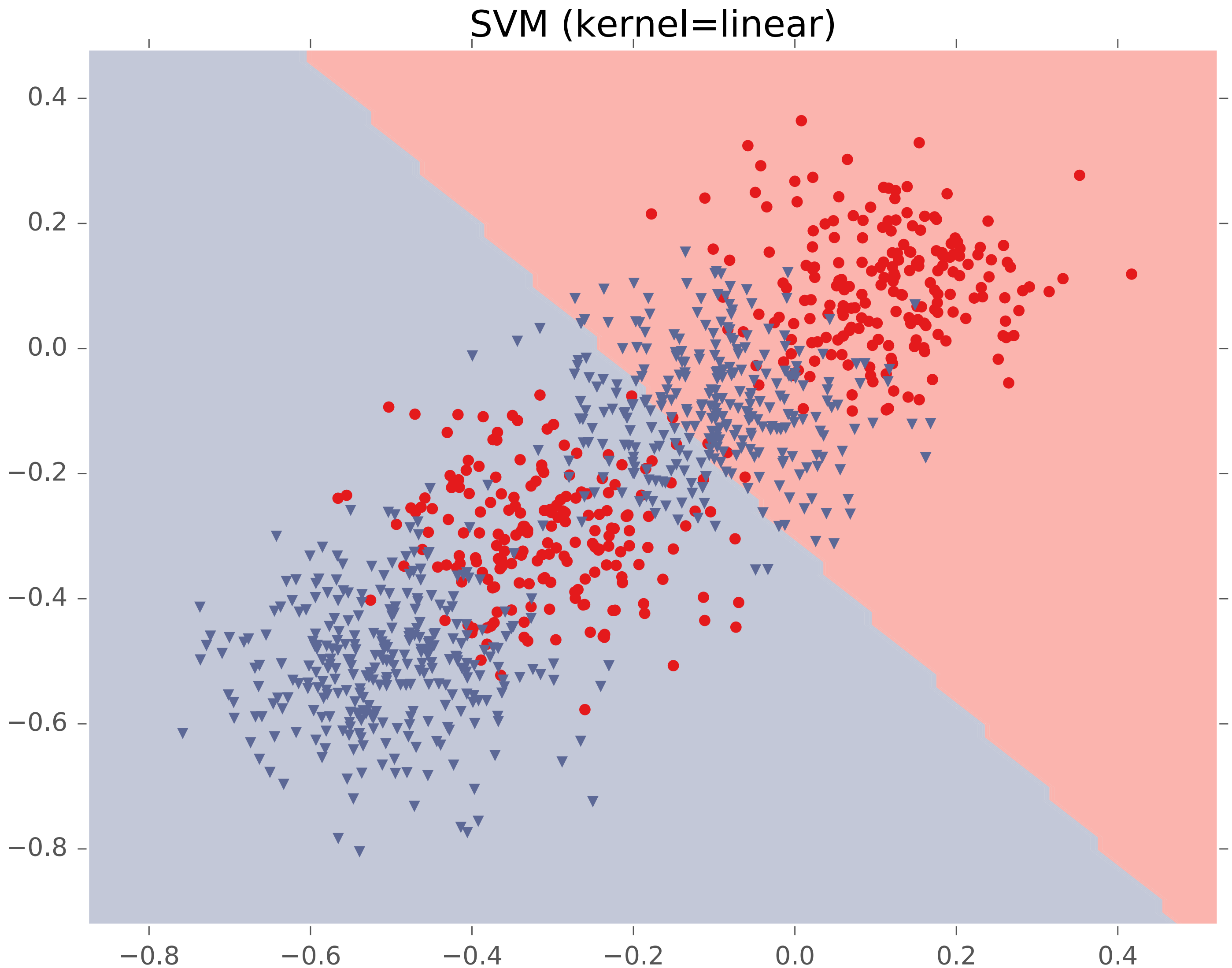

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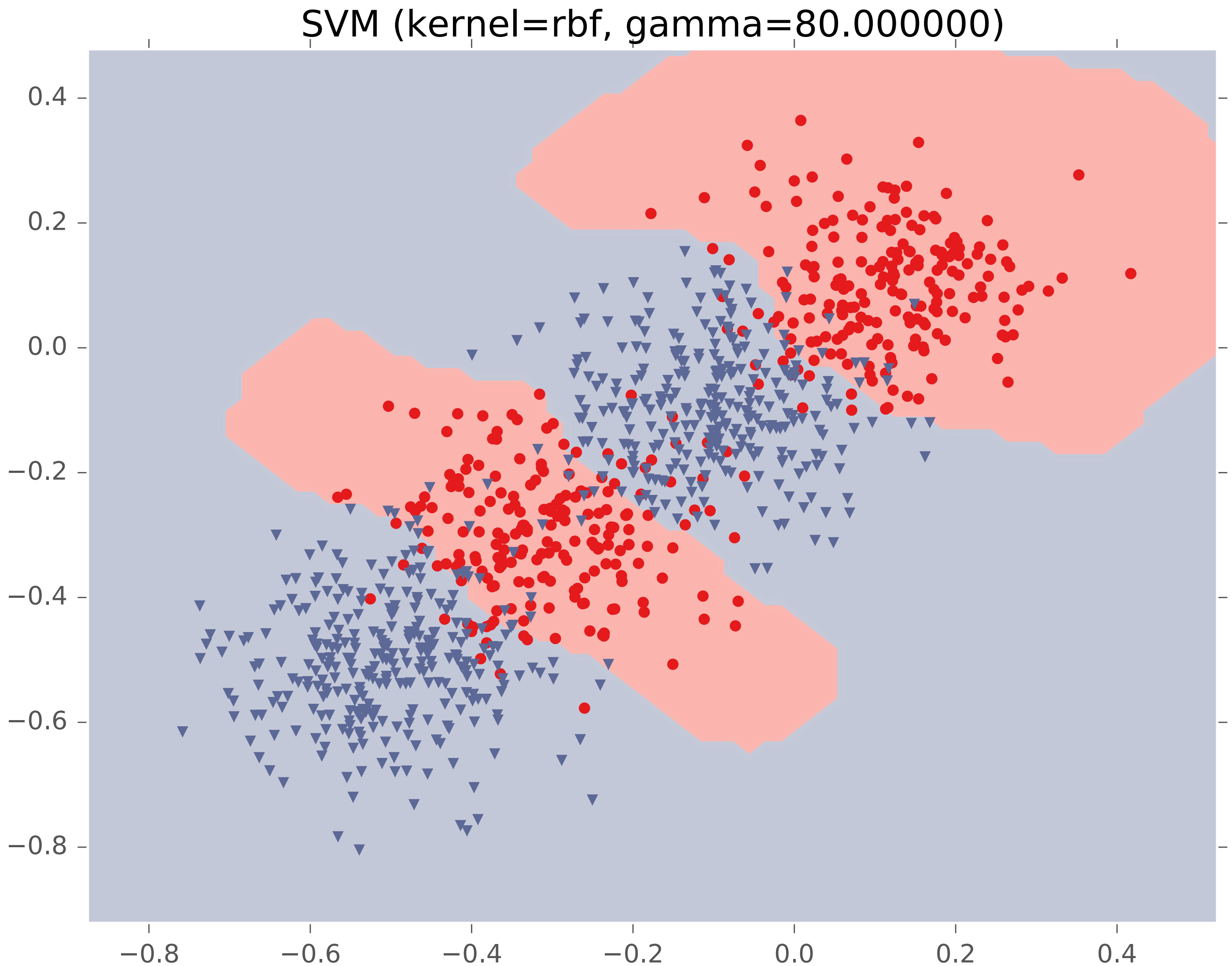

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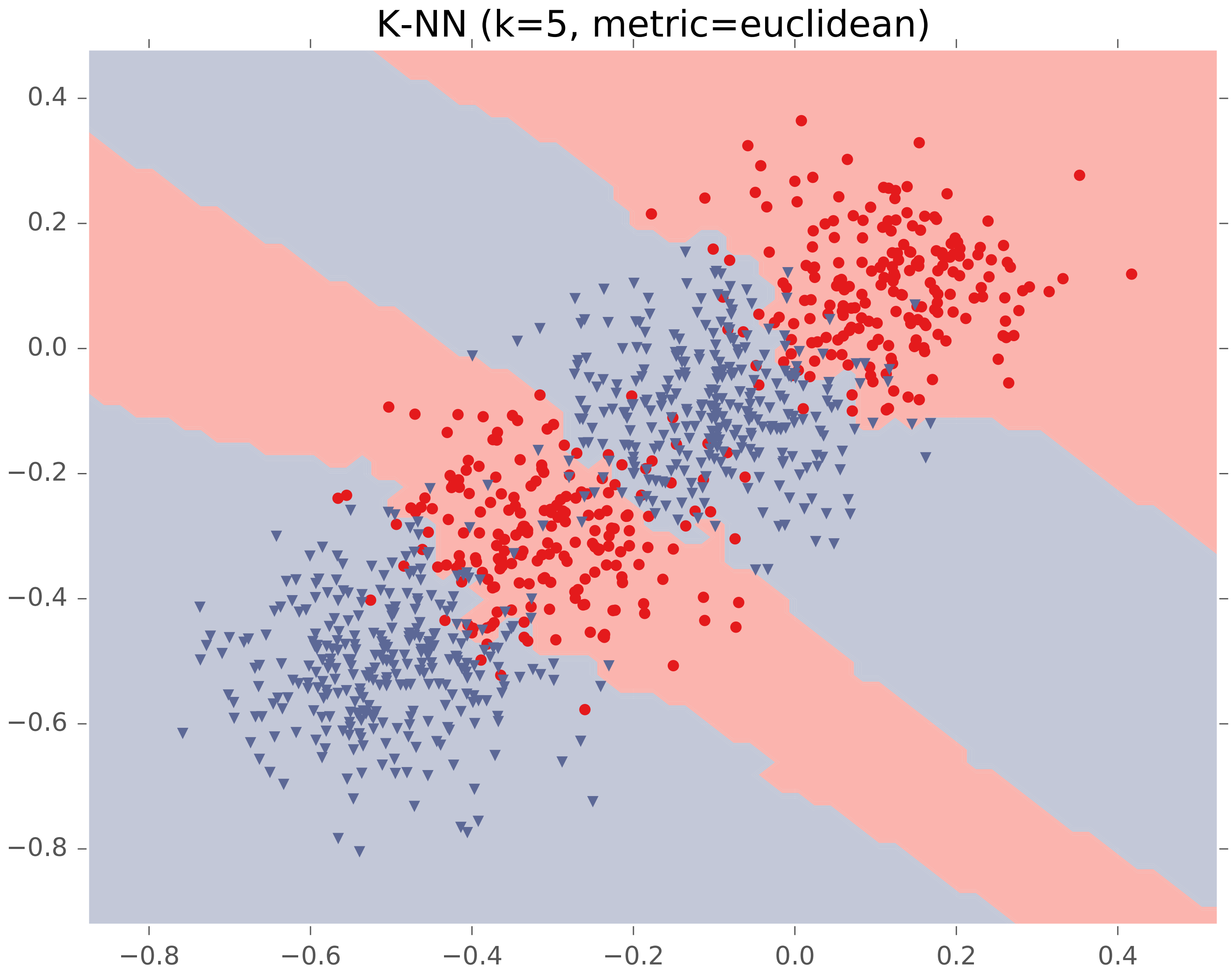

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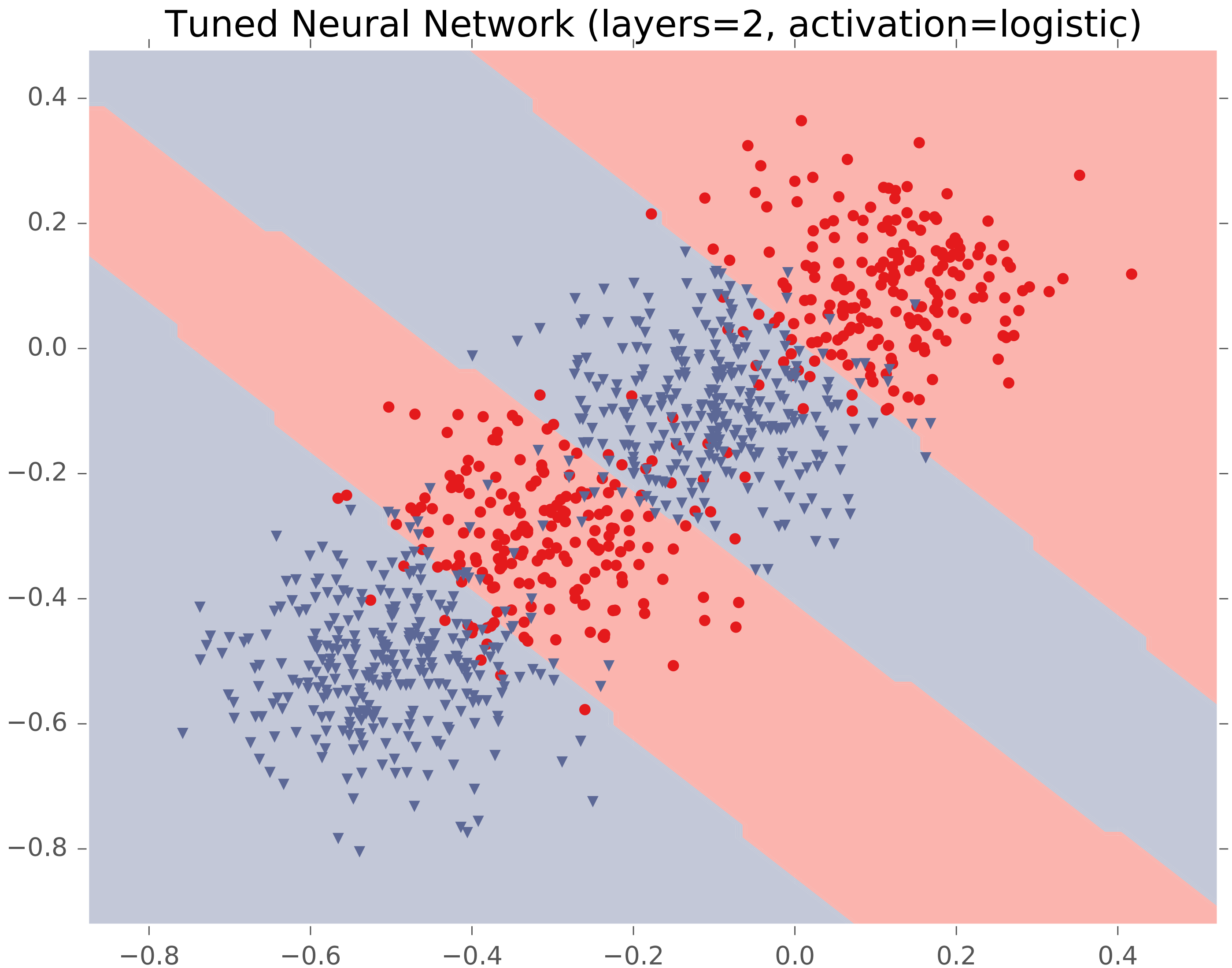

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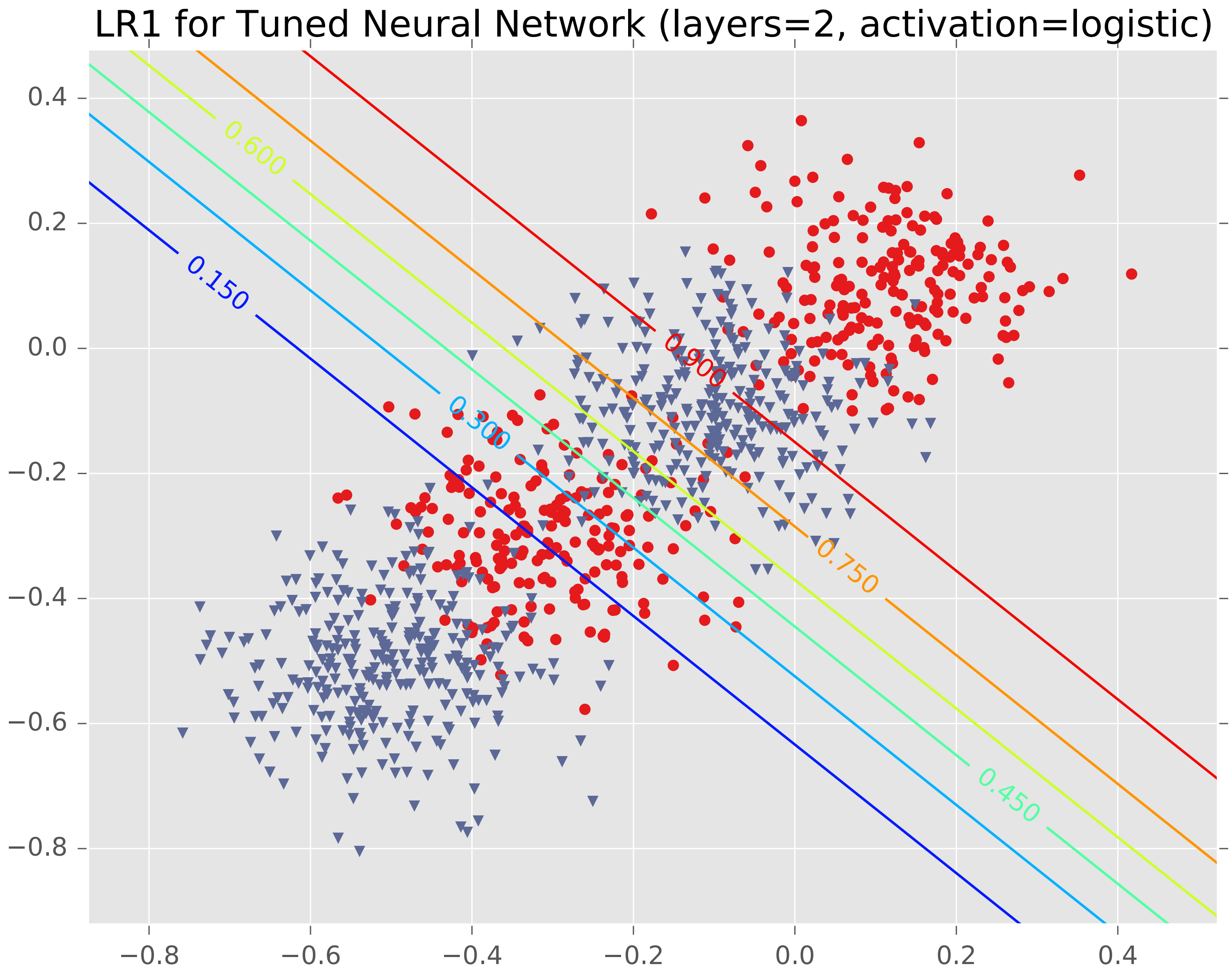

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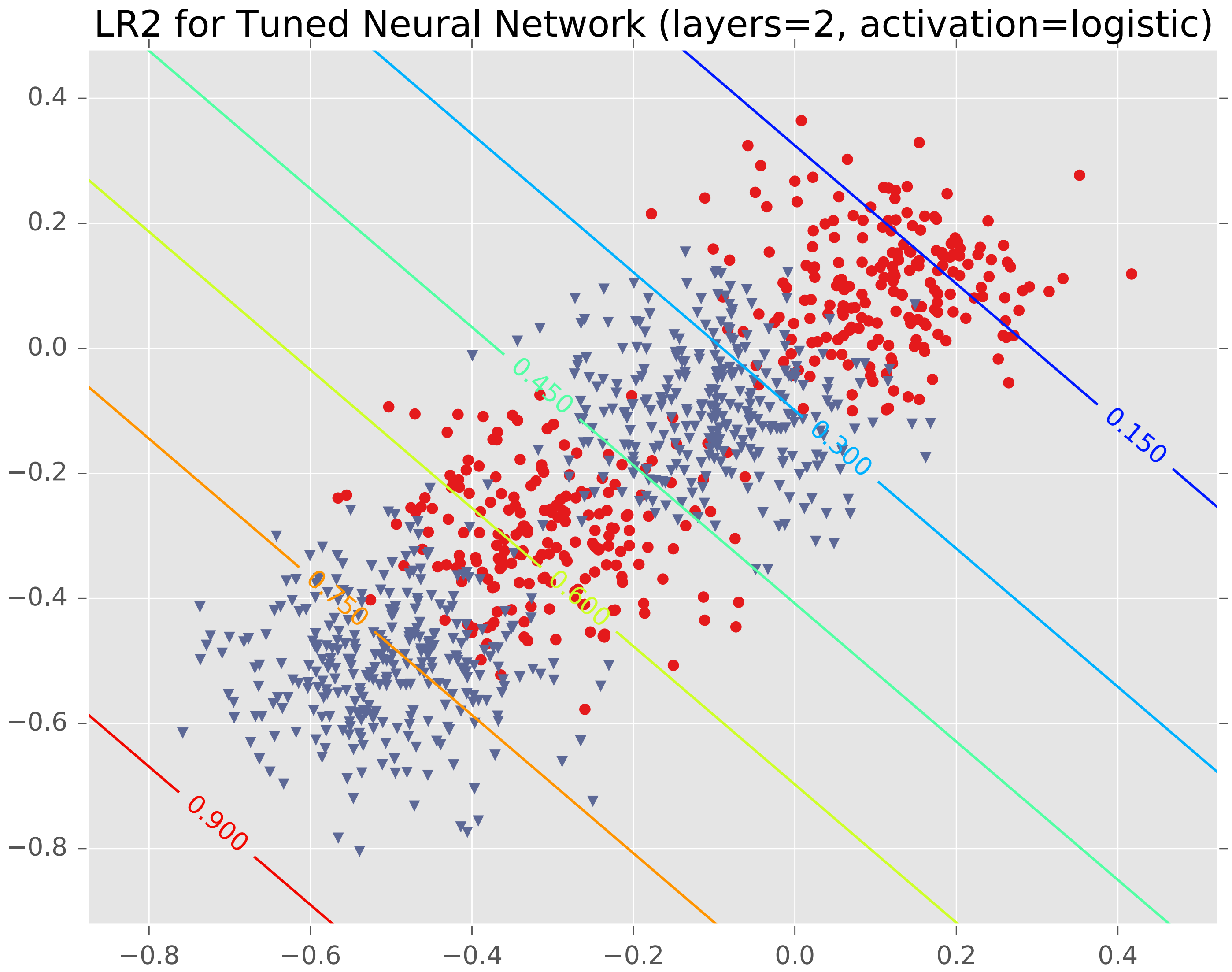

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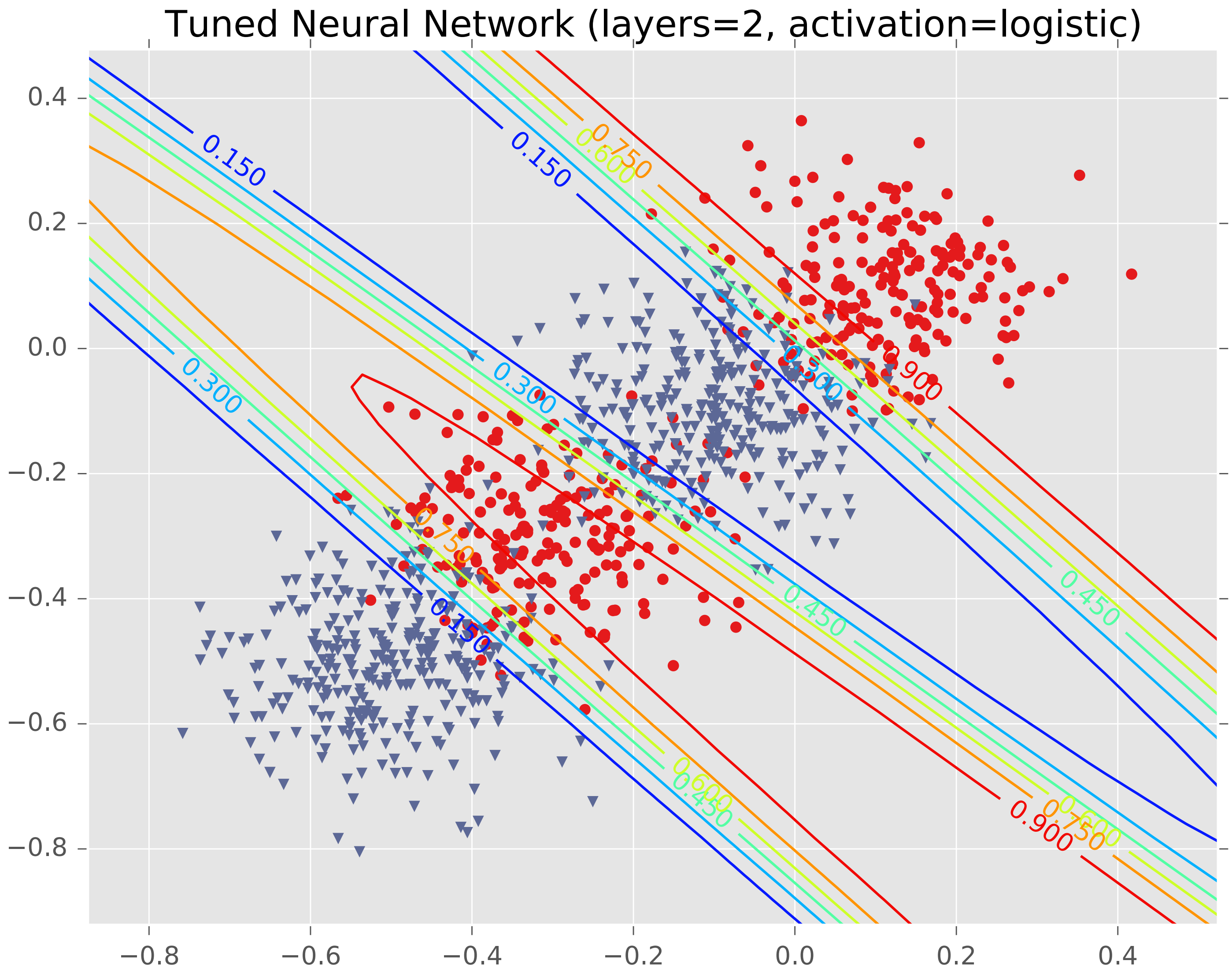

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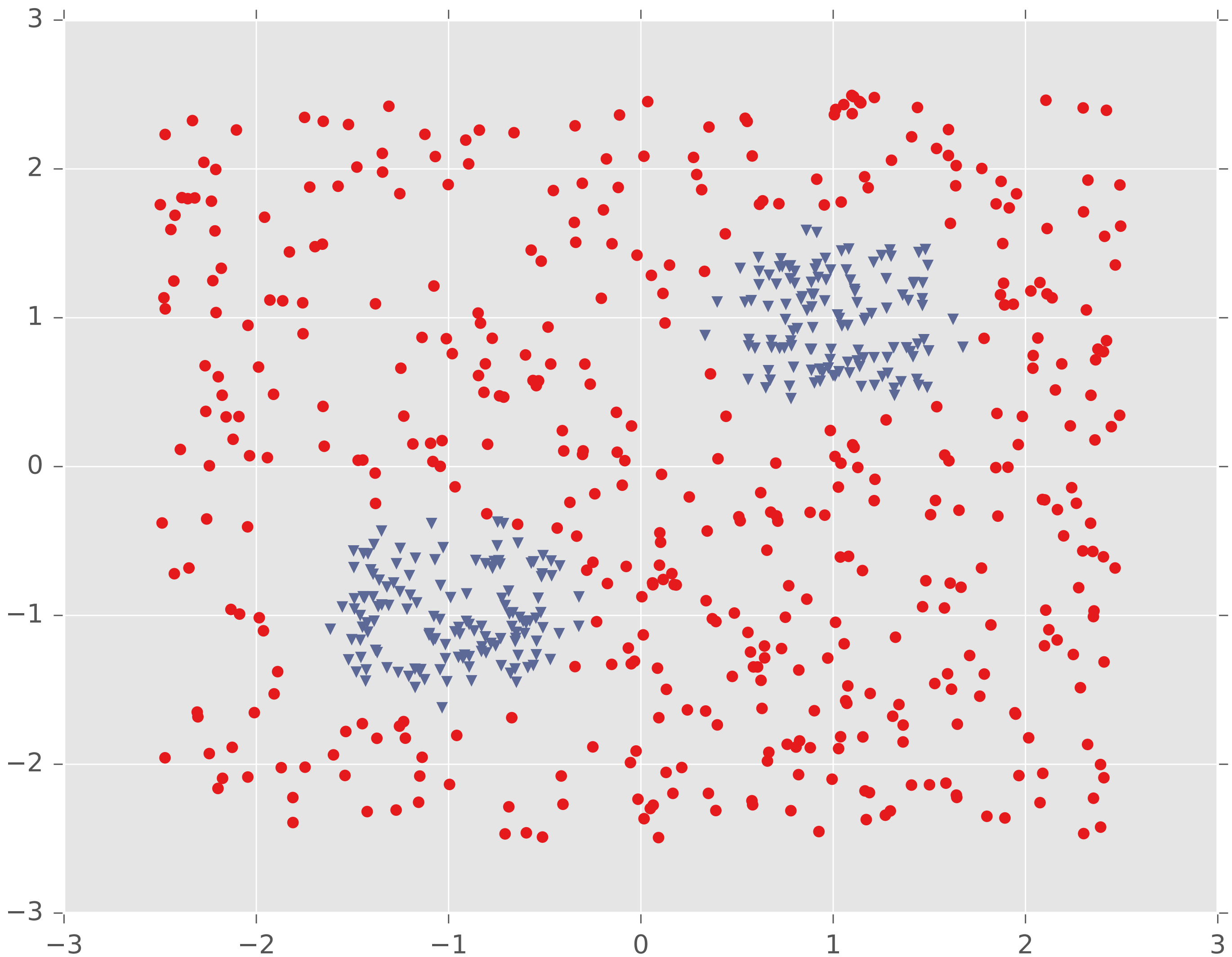

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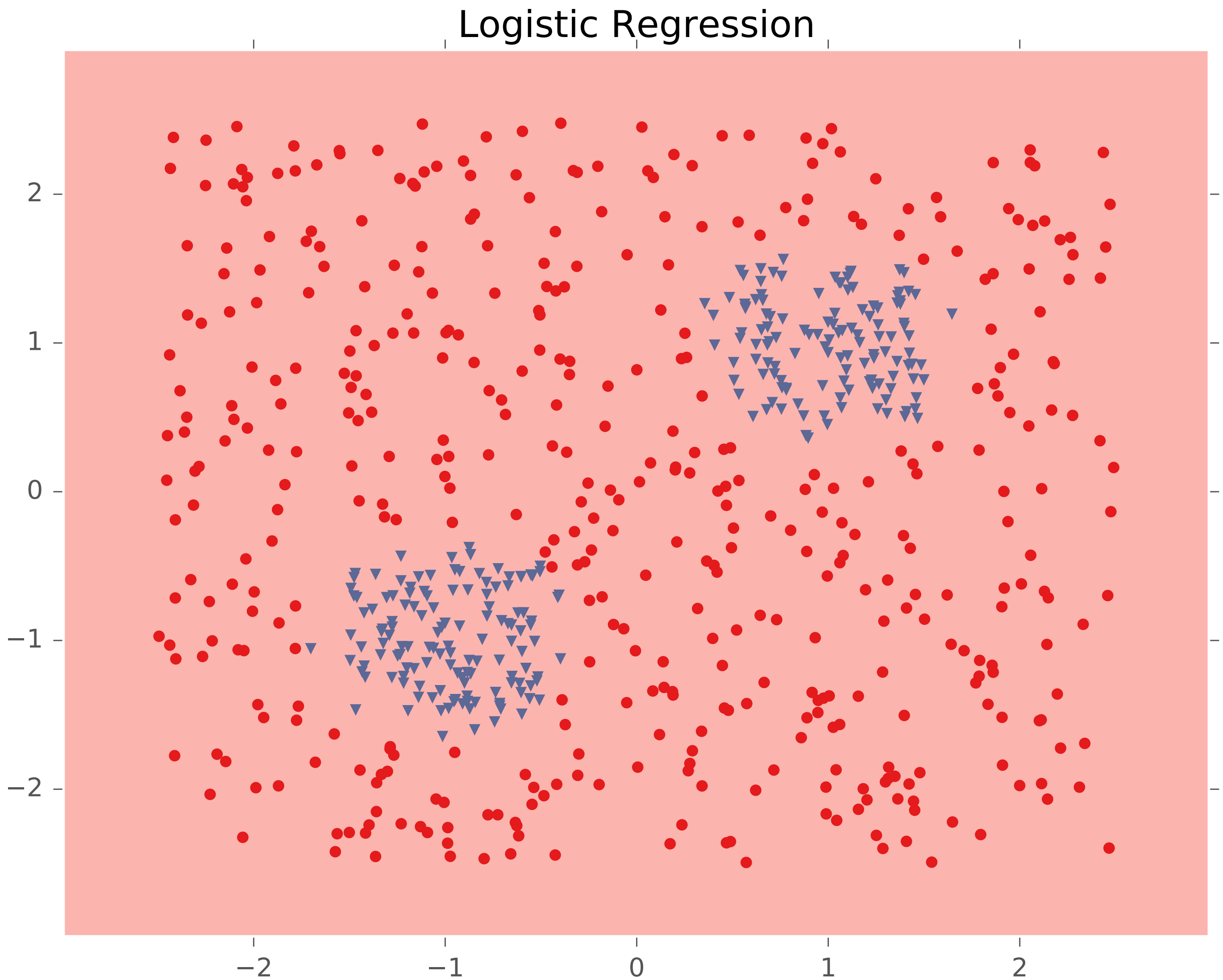

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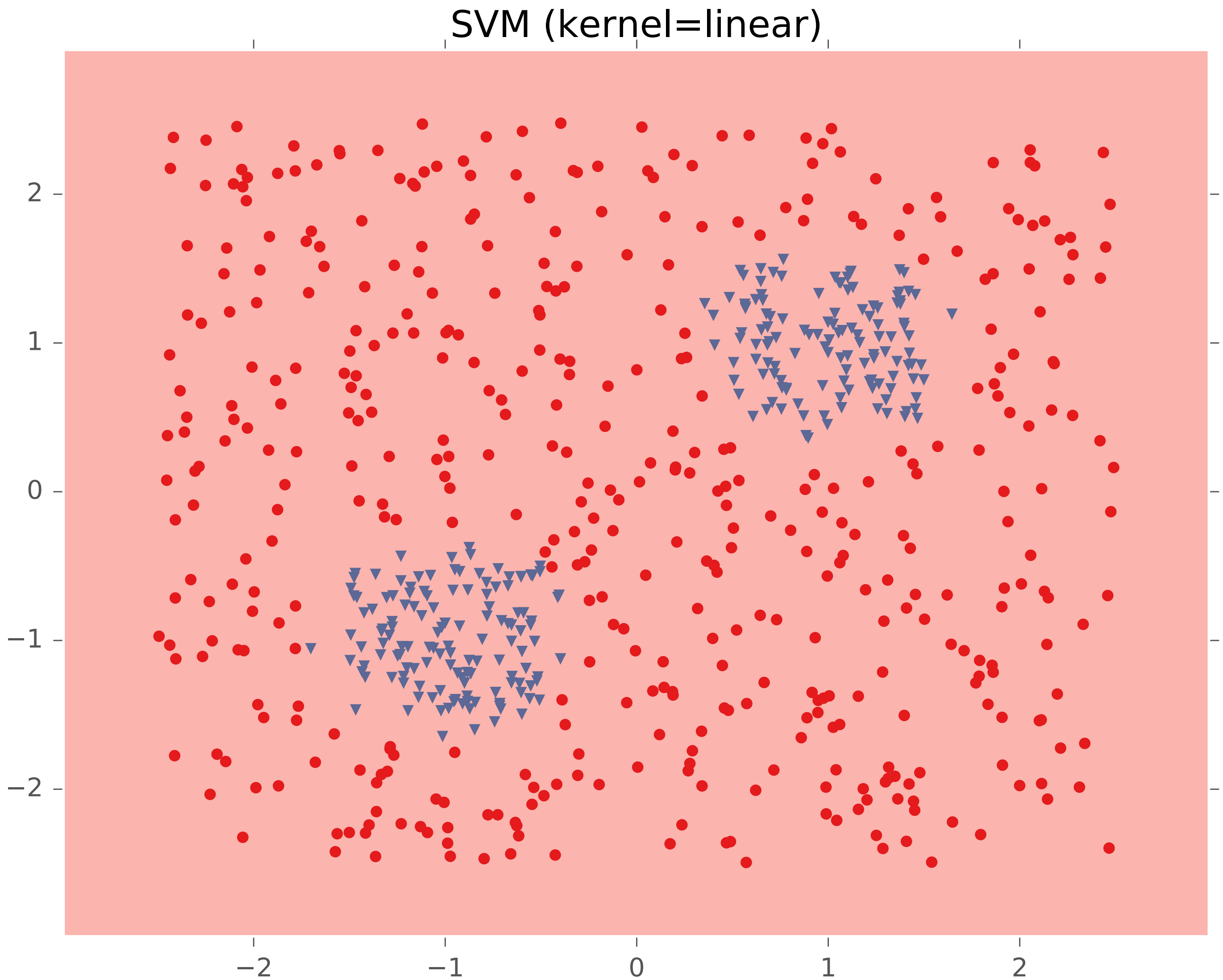

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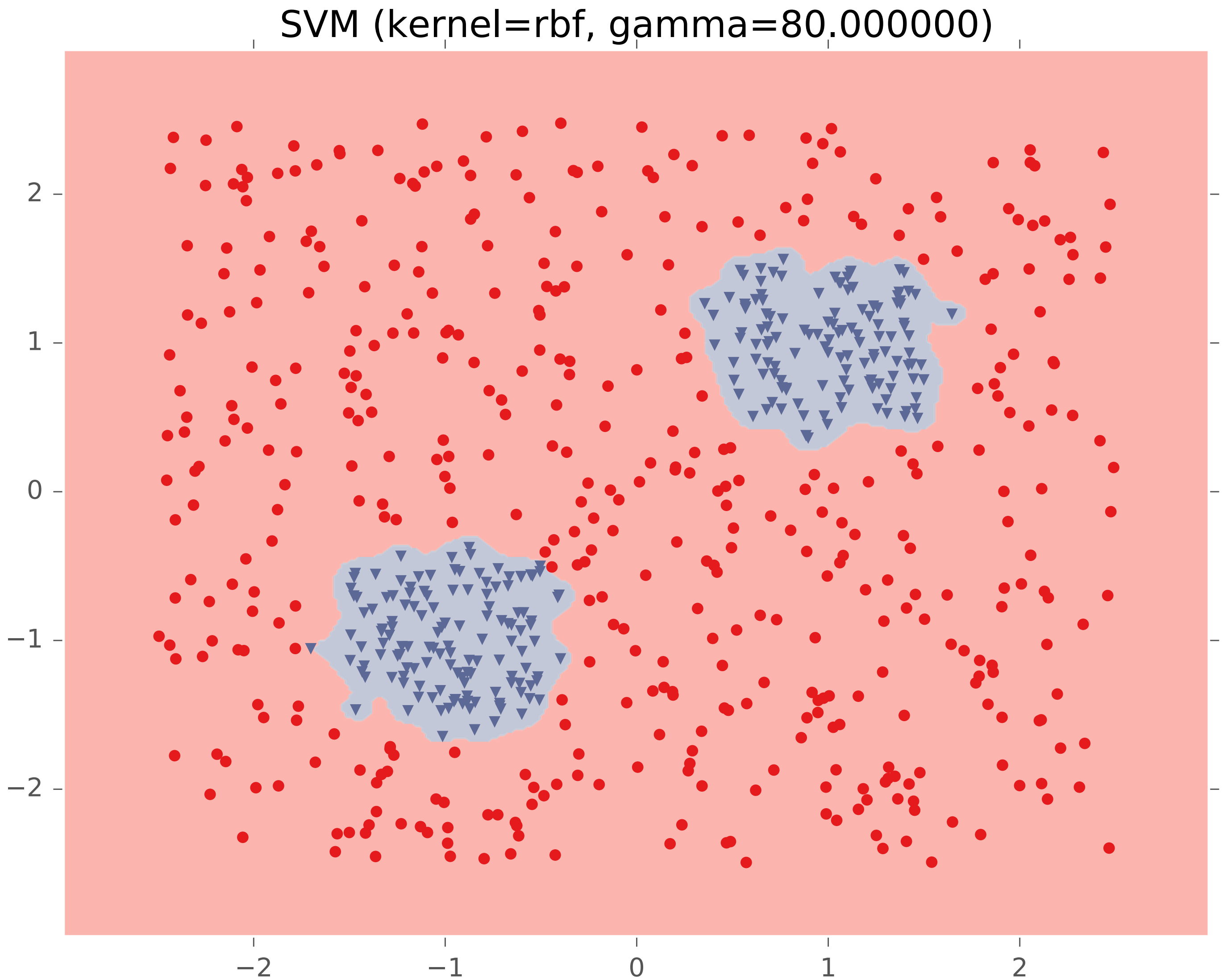

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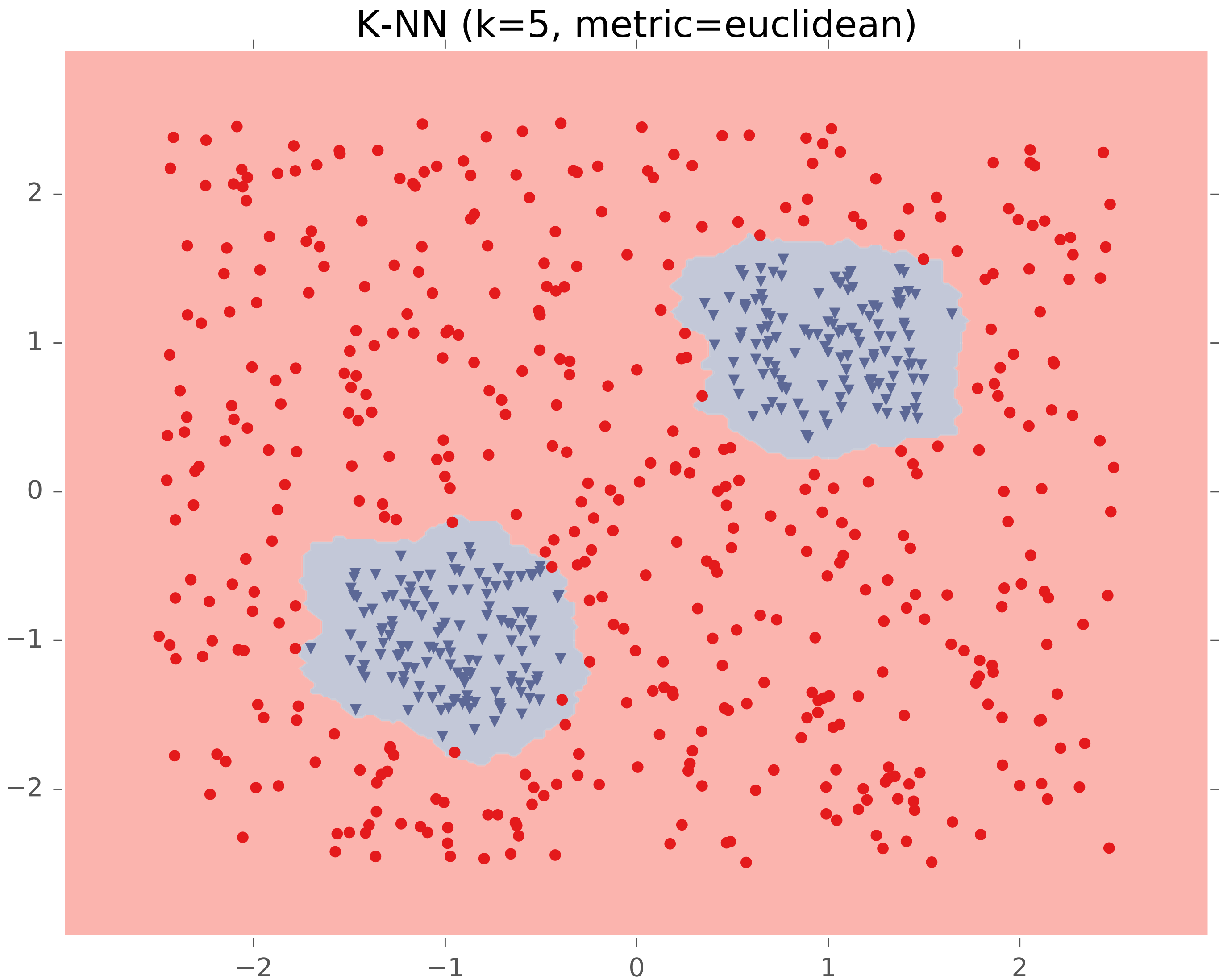

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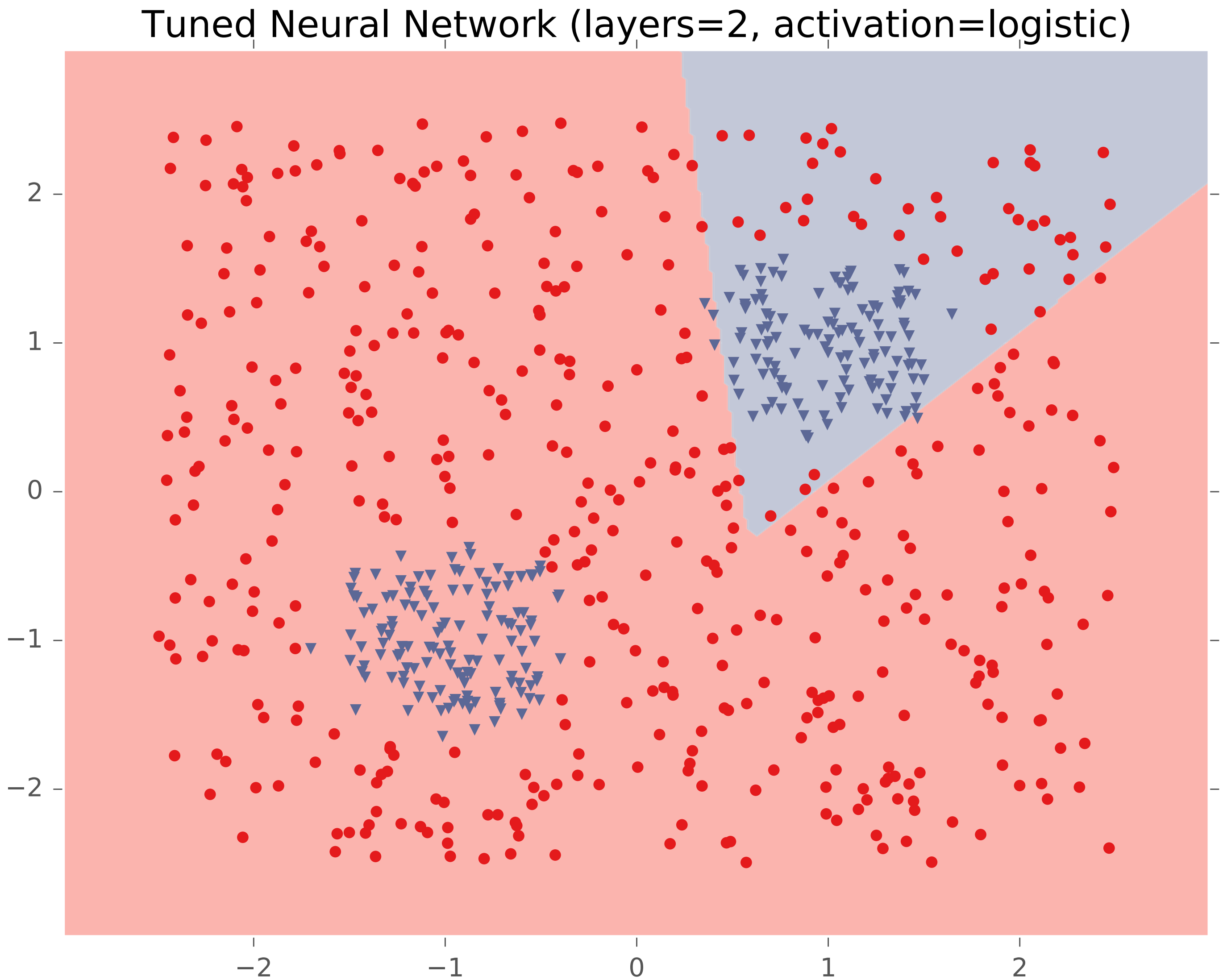

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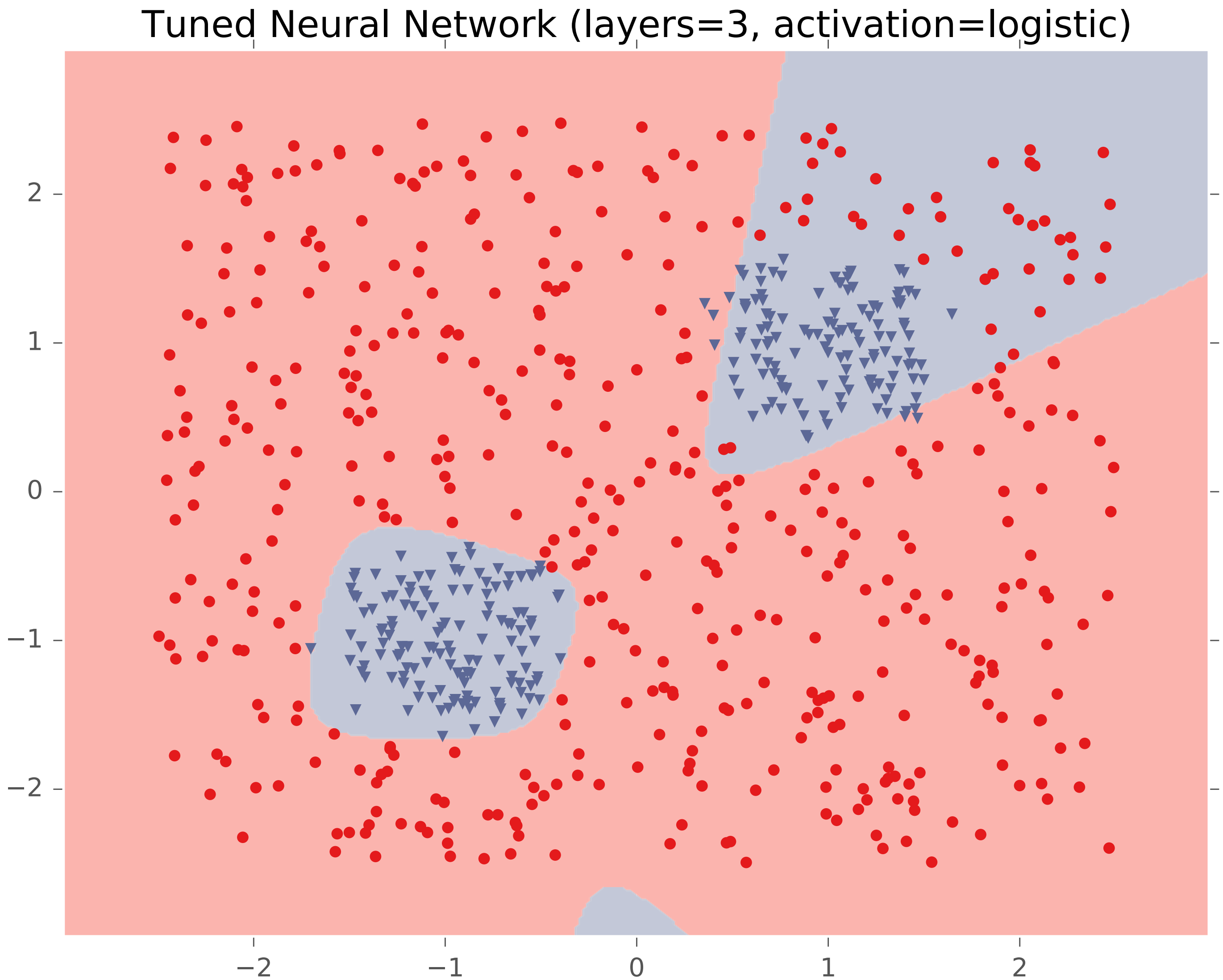

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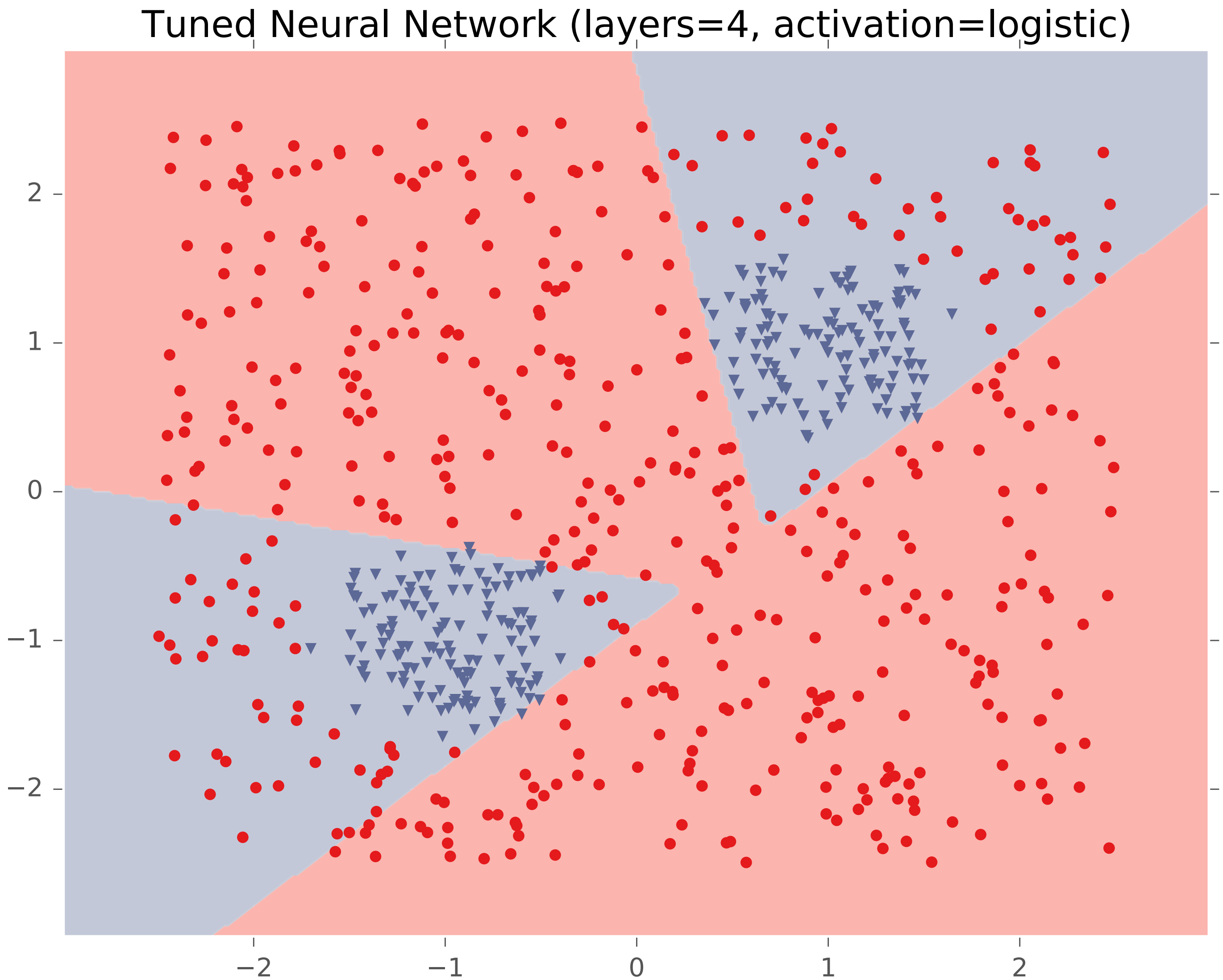

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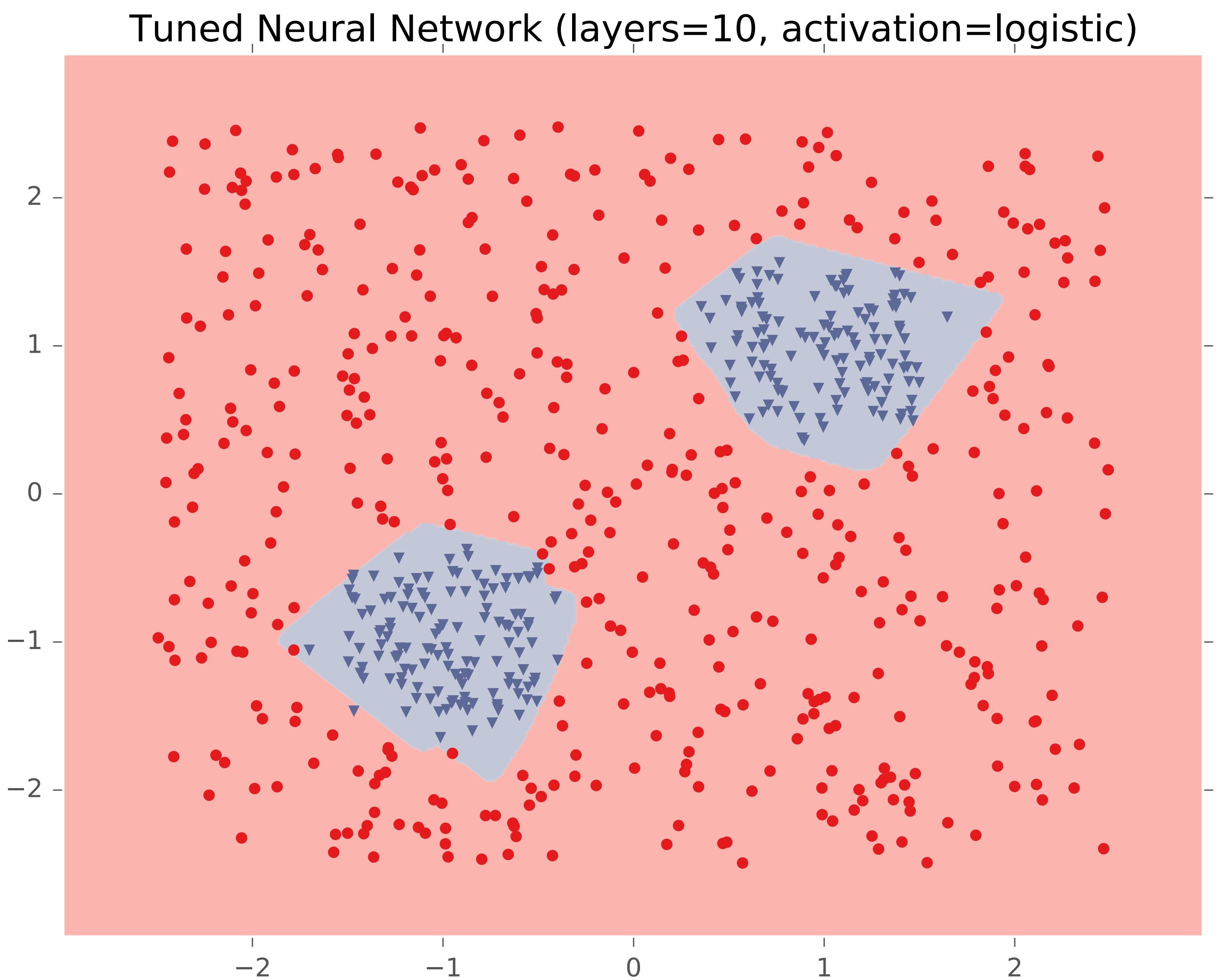


ARCHITECTURES

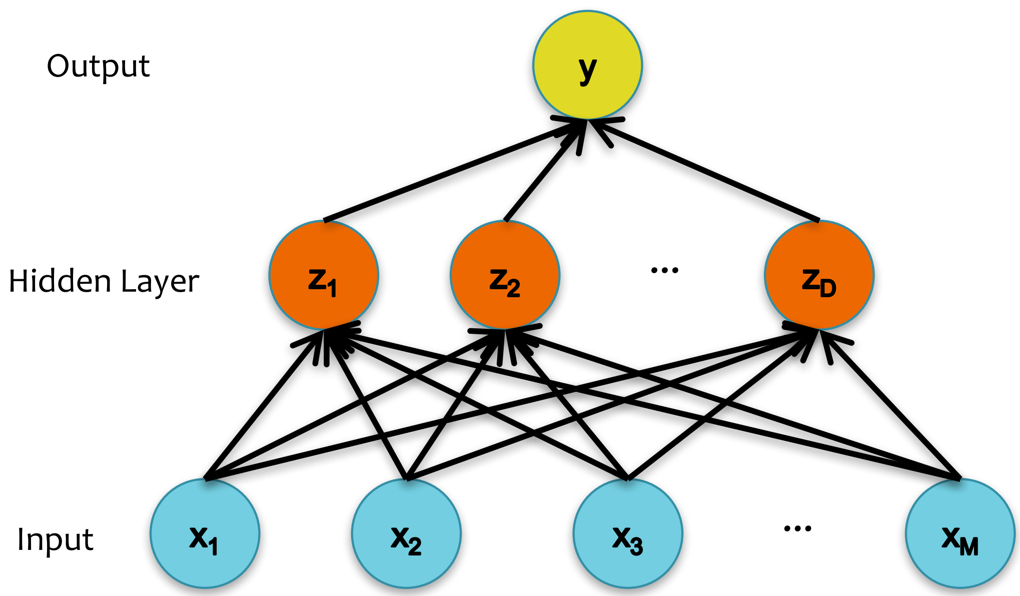
Neural Network Architectures

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

Activation Functions

Neural Network with sigmoid activation functions



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

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

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

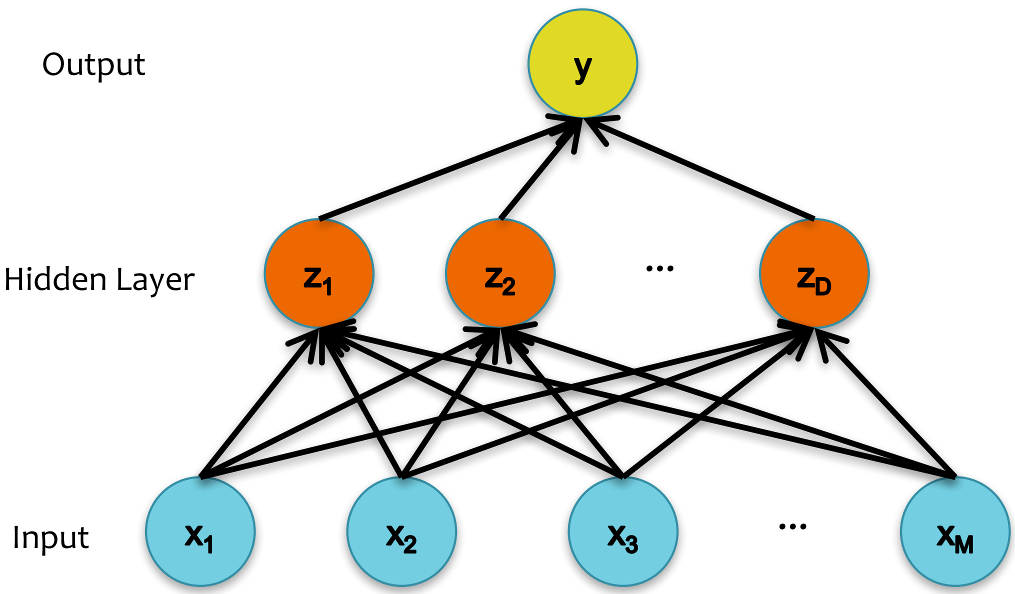
(C) Hidden (sigmoid)
$z_j = \frac{1}{1+\exp(-a_j)}, \ \forall j$

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

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

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

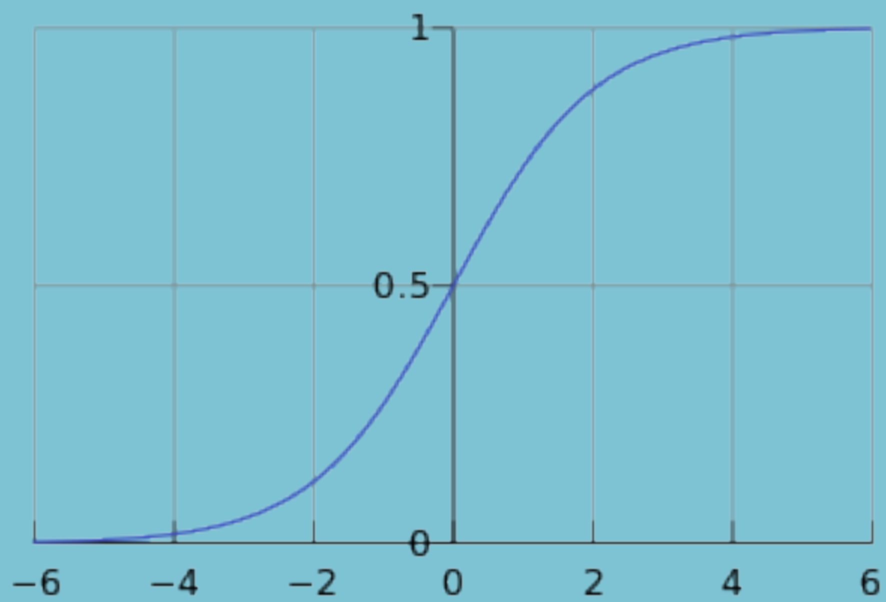
(B) **Hidden (linear)**
$a_j = \sum_{i=0}^{M} \alpha_{ji} x_i, \ \forall j$

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

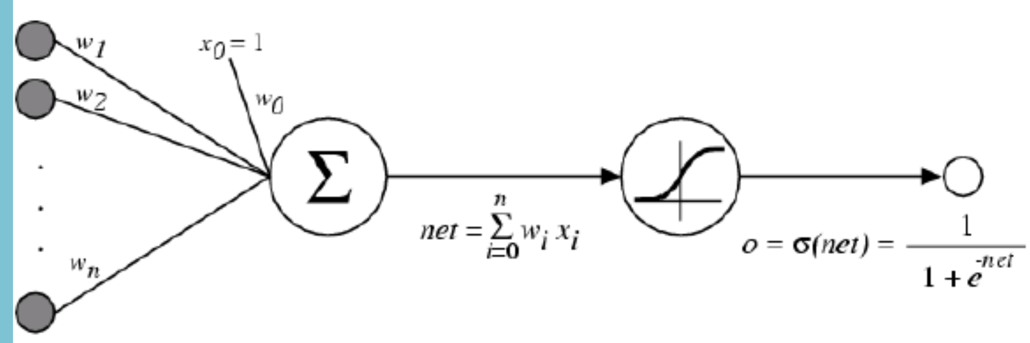
Activation Functions

Sigmoid / Logistic Function

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

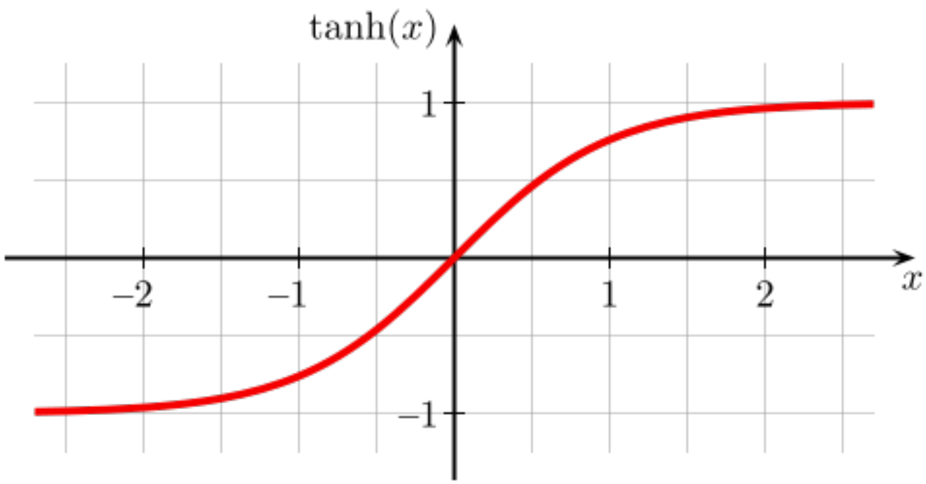


So far, we've assumed that the activation function (nonlinearity) is always the sigmoid function…



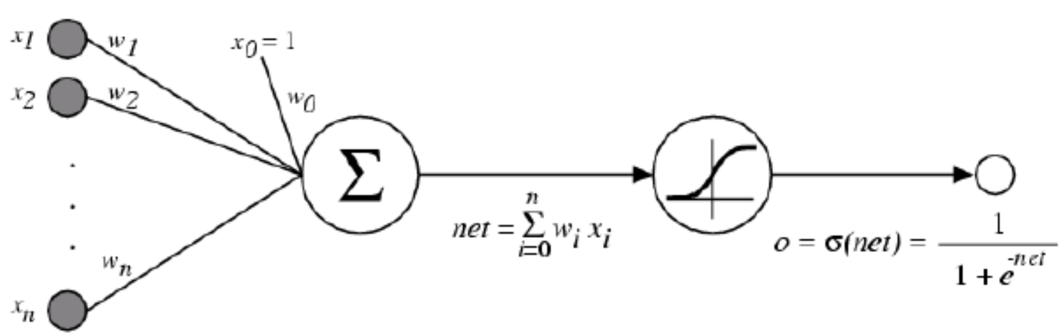
Activation Functions

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



Alternate 1: tanh

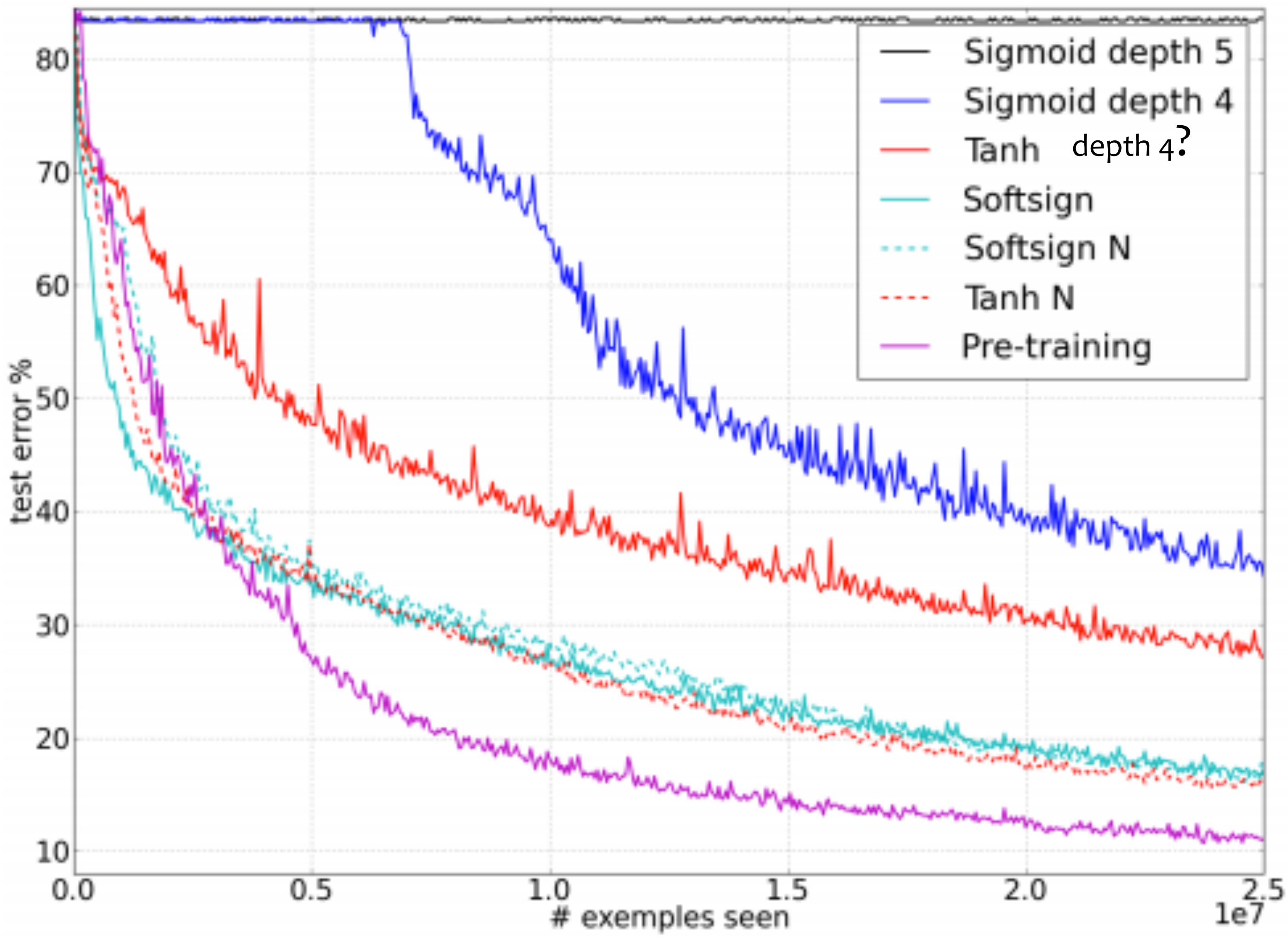
Like logistic function but shifted to range [-1, +1]



Slide from William Cohen

Understanding the difficulty of training deep feedforward neural networks

AI Stats 2010

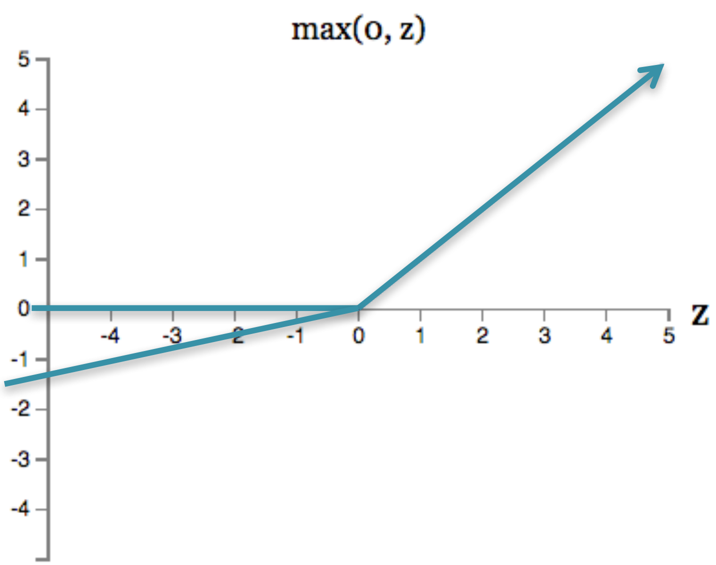


sigmoid
vs.
tanh

Figure from Glorot & Bentio (2010)

Activation Functions

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

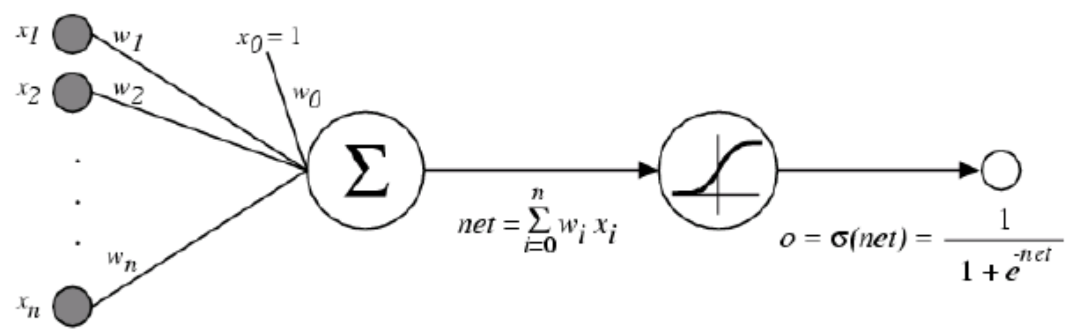


Alternate 2: rectified linear unit

Linear with a cutoff at zero

(Implementation: clip the gradient when you pass zero)

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



Slide from William Cohen

Activation Functions

- A new change: modifying the nonlinearity
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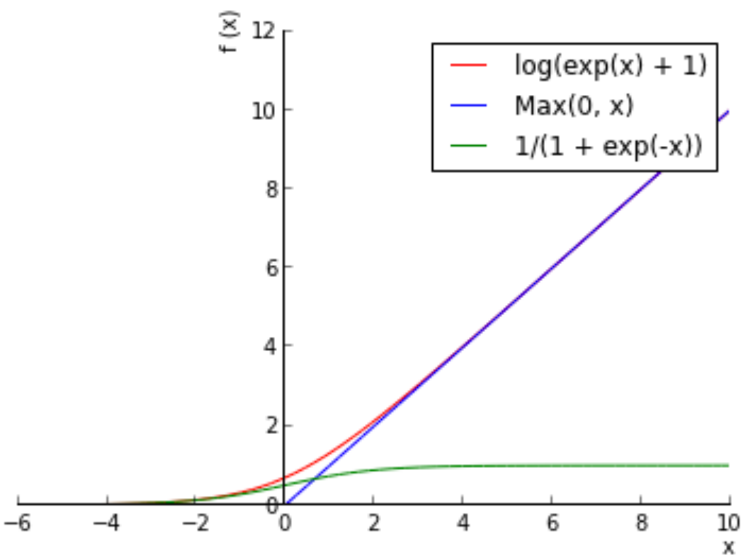
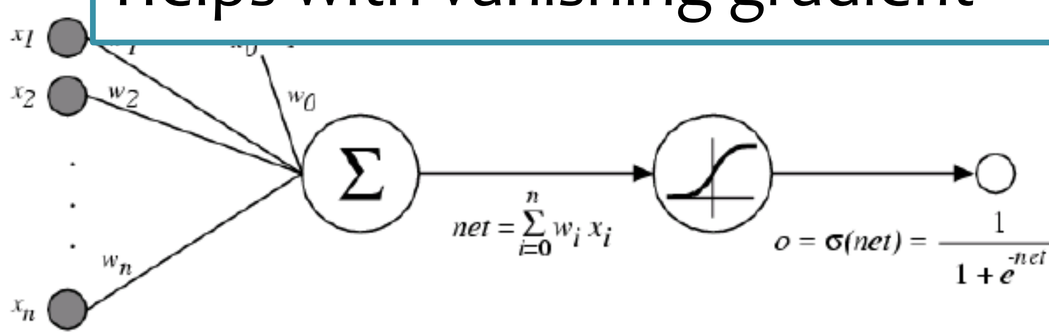


Alternate 2: rectified linear unit

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

- Regression:
  - Use the same objective as Linear Regression
  - Quadratic loss (i.e. mean squared error)
- Classification:
  - Use the same objective as Logistic Regression
  - Cross-entropy (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	$J = y^* \log(y) + (1 - y^*) \log(1 - y)$	$\frac{dJ}{dy} = y^* \frac{1}{y} + (1 - y^*) \frac{1}{y - 1}$

Cross-entropy vs. Quadratic loss

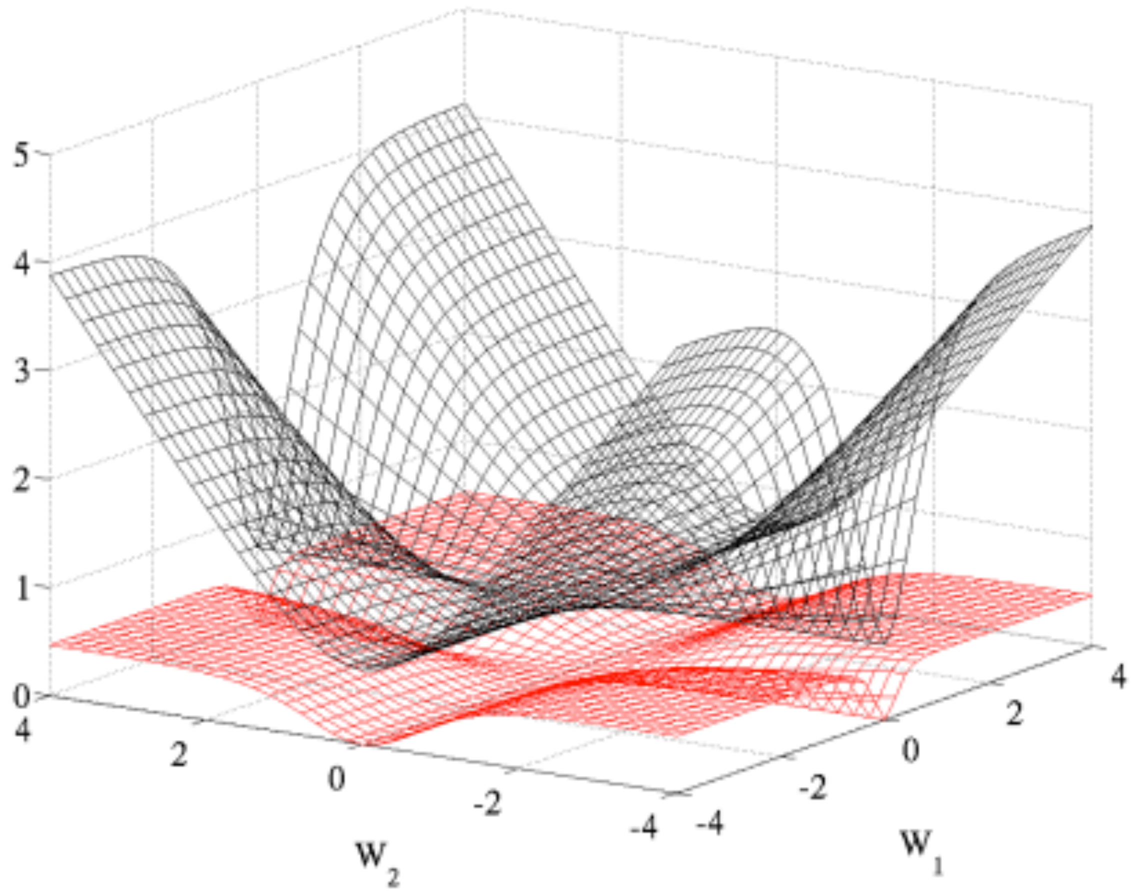


Figure 5: *Cross entropy (black, surface on top) and quadratic (red, bottom surface) cost as a function of two weights (one at each layer) of a network with two layers, W_1 respectively on the first layer and W_2 on the second, output layer.*

Figure from Glorot & Bentio (2010)

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)

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

Objective Functions

Matching Quiz: Suppose you are given a neural net with a single output, y, and one hidden layer.

1) Minimizing sum of squared errors…	…gives…	5) …MLE estimates of weights assuming target follows a Bernoulli with parameter given by the output value
2) Minimizing sum of squared errors plus squared Euclidean norm of weights…		6) …MAP estimates of weights assuming weight priors are zero mean Gaussian
3) Minimizing cross-entropy…		7) …estimates with a large margin on the training data
4) Minimizing hinge loss…		8) …MLE estimates of weights assuming zero mean Gaussian noise on the output value

A. 1=5, 2=7, 3=6, 4=8
B. 1=5, 2=7, 3=8, 4=6
C. 1=7, 2=5, 3=5, 4=7
D. 1=7, 2=5, 3=6, 4=8
E. 1=8, 2=6, 3=5, 4=7
F. 1=8, 2=6, 3=8, 4=6

BACKPROPAGATION

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

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

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

Training

Approaches to Differentiation

- **Question 1:**
  When can we compute the gradients of the parameters of an arbitrary neural network?

- **Question 2:**
  When can we make the gradient computation efficient?

Training

Approaches to Differentiation

Given $f : \mathbb{R}^A \rightarrow \mathbb{R}^B, f(\mathbf{x})$

Compute $\frac{\partial f(\mathbf{x})_i}{\partial x_j} \forall i, j$

1. Finite Difference Method
   - Pro: Great for testing implementations of backpropagation
   - Con: Slow for high dimensional inputs / outputs
   - Required: Ability to call the function f($\mathbf{x}$) on any input $\mathbf{x}$
2. Symbolic Differentiation
   - Note: The method you learned in high-school
   - Note: Used by Mathematica / Wolfram Alpha / Maple
   - Pro: Yields easily interpretable derivatives
   - Con: Leads to exponential computation time if not carefully implemented
   - Required: Mathematical expression that defines f($\mathbf{x}$)
3. Automatic Differentiation - Reverse Mode
   - Note: Called *Backpropagation* when applied to Neural Nets
   - Pro: Computes partial derivatives of one output $f(\mathbf{x})_i$ with respect to all inputs x_j in time proportional to computation of f($\mathbf{x}$)
   - Con: Slow for high dimensional outputs (e.g. vector-valued functions)
   - Required: Algorithm for computing f($\mathbf{x}$)
4. Automatic Differentiation - Forward Mode
   - Note: Easy to implement. Uses dual numbers.
   - Pro: Computes partial derivatives of all outputs $f(\mathbf{x})_i$ with respect to one input x_j in time proportional to computation of f($\mathbf{x}$)
   - Con: Slow for high dimensional inputs (e.g. vector-valued $\mathbf{x}$)
   - Required: Algorithm for computing f($\mathbf{x}$)

Finite Difference Method

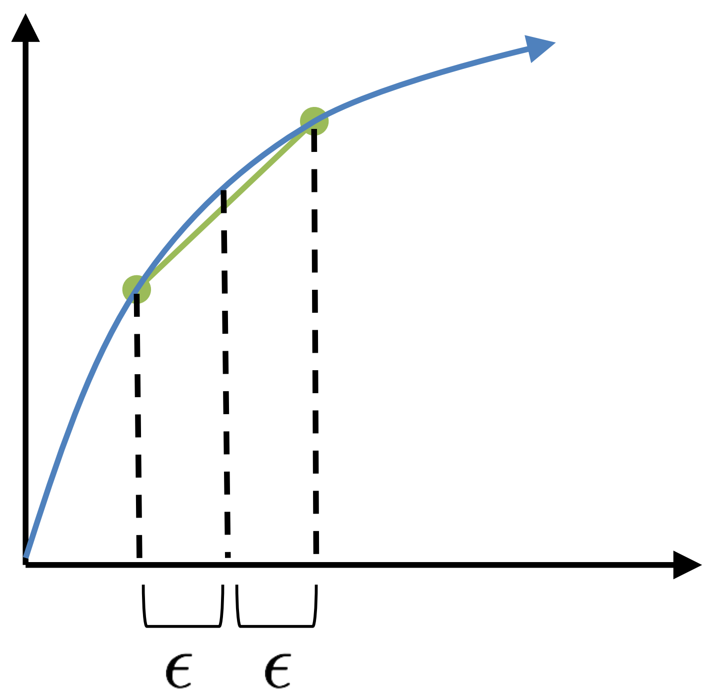
The *centered* finite difference approximation is:

$$\frac{\partial}{\partial \theta_i} J(\boldsymbol{\theta}) \approx \frac{(J(\boldsymbol{\theta} + \epsilon \cdot \boldsymbol{d}_i) - J(\boldsymbol{\theta} - \epsilon \cdot \boldsymbol{d}_i))}{2\epsilon} \tag{1}$$

where $\boldsymbol{d}_i$ is a 1-hot vector consisting of all zeros except for the ith entry of $\boldsymbol{d}_i$, which has value 1.

Notes:

- Suffers from issues of floating point precision, in practice
- Typically only appropriate to use on small examples with an appropriately chosen epsilon



Symbolic Differentiation

Calculus Quiz #1:

Suppose x = 2 and z = 3, what are dy/dx and dy/dz for the function below?

$$y = \exp(xz) + \frac{xz}{\log(x)} + \frac{\sin(\log(x))}{\exp(xz)}$$

Calculus Quiz #2:

A neural network with 2 hidden layers can be written as:

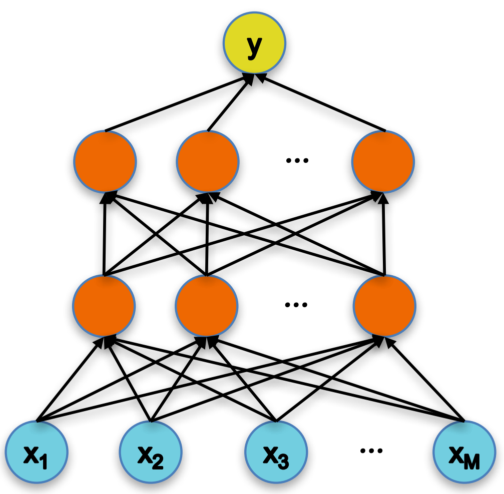
$$y = \sigma(\boldsymbol{\beta}^T \sigma((\boldsymbol{\alpha}^{(2)})^T \sigma((\boldsymbol{\alpha}^{(1)})^T \mathbf{x}))$$

where $y \in \mathbb{R}$, $\mathbf{x} \in \mathbb{R}^{D^{(0)}}$, $\boldsymbol{\beta} \in \mathbb{R}^{D^{(2)}}$ and $\boldsymbol{\alpha}^{(i)}$ is a $D^{(i)} \times D^{(i-1)}$ matrix. Nonlinear functions are applied elementwise:

$$\sigma(\mathbf{a}) = [\sigma(a_1), \ldots, \sigma(a_K)]^T$$

Let σ be sigmoid: $\sigma(a) = \frac{1}{1+exp-a}$

What is $\frac{\partial y}{\partial \beta_j}$ and $\frac{\partial y}{\partial \alpha_j^{(i)}}$ for all i, j.



Training

Chain Rule

Whiteboard

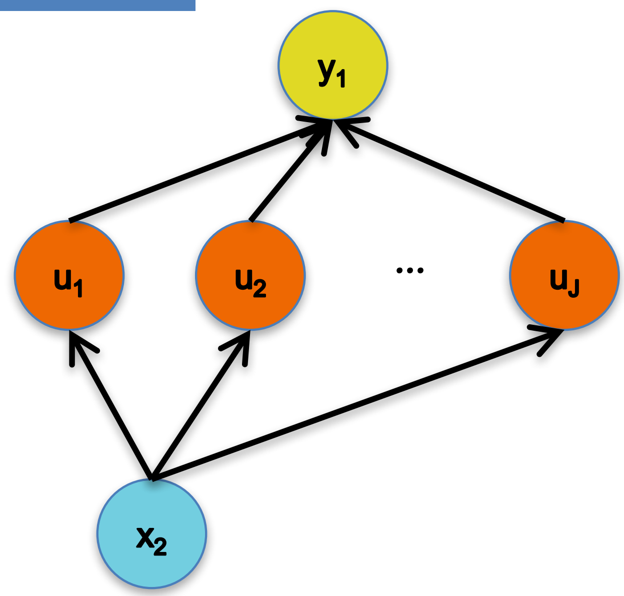
- Chain Rule of Calculus

Chain Rule

Given: $\boldsymbol{y} = g(\boldsymbol{u})$ and $\boldsymbol{u} = h(\boldsymbol{x})$.

Chain Rule:

$$\frac{dy_i}{dx_k} = \sum_{j=1}^{J} \frac{dy_i}{du_j}\frac{du_j}{dx_k}, \qquad \forall i, k$$



Training

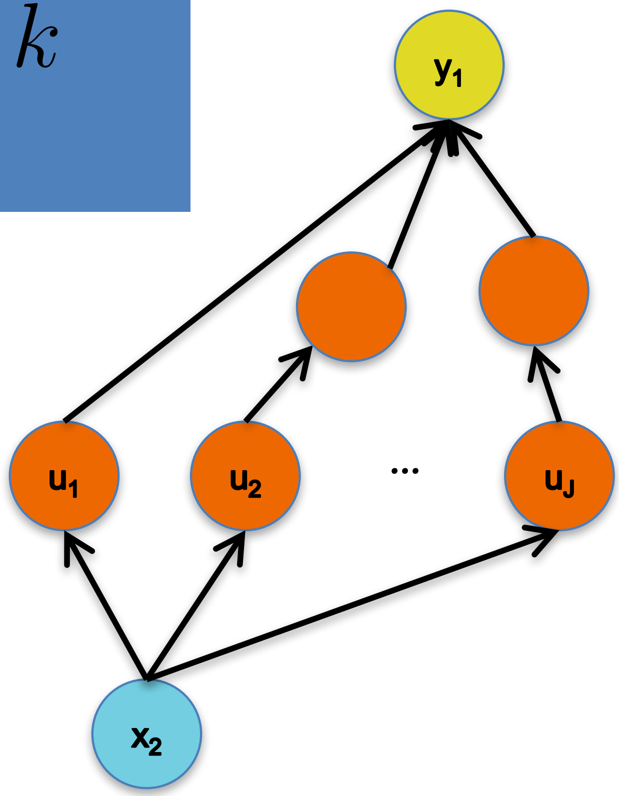
Chain Rule

Given: $\boldsymbol{y} = g(\boldsymbol{u})$ and $\boldsymbol{u} = h(\boldsymbol{x})$.

Chain Rule:

$$\frac{dy_i}{dx_k} = \sum_{j=1}^{J} \frac{dy_i}{du_j}\frac{du_j}{dx_k}, \quad \forall i, k$$

Backpropagation is just repeated application of the **chain rule** from Calculus 101.



Training

Backpropagation

Whiteboard

- Example: Backpropagation for Calculus Quiz #1

Calculus Quiz #1:

Suppose x = 2 and z = 3, what are dy/dx and dy/dz for the function below?

$$y = \exp(xz) + \frac{xz}{\log(x)} + \frac{\sin(\log(x))}{\exp(xz)}$$

Backpropagation

Automatic Differentiation – Reverse Mode (aka. Backpropagation)

<u>Forward Computation</u>

1. Write an **algorithm** for evaluating the function $y = f(\mathbf{x})$. The algorithm defines a **directed acyclic graph**, where each variable is a node (i.e. the "**computation graph**")
2. Visit each node in **topological order**.
   For variable u_i with inputs $v_1, \ldots, v_N$
   a. Compute $u_i = g_i(v_1, \ldots, v_N)$
   b. Store the result at the node

<u>Backward Computation</u>

1. **Initialize** all partial derivatives dy/du_j to 0 and $dy/dy = 1$.
2. Visit each node in **reverse topological order**.
   For variable $u_i = g_i(v_1, \ldots, v_N)$
   a. We already know dy/du_i
   b. Increment dy/dv_j by $(dy/du_i)(du_i/dv_j)$
   (Choice of algorithm ensures computing (du_i/dv_j) is easy)

Return partial derivatives dy/du_i for all variables

Backpropagation

Simple Example: The goal is to compute $J = \cos(\sin(x^2) + 3x^2)$ on the forward pass and the derivative $\frac{dJ}{dx}$ on the backward pass.

Forward

$J = cos(u)$

$u = u_1 + u_2$

$u_1 = sin(t)$

$u_2 = 3t$

$t = x^2$

Training

Backpropagation

Simple Example: The goal is to compute $J = \cos(\sin(x^2) + 3x^2)$ on the forward pass and the derivative $\frac{dJ}{dx}$ on the backward pass.

Forward	Backward
$J = cos(u)$	$\frac{dJ}{du} \mathrel{+}= -sin(u)$
$u = u_1 + u_2$	$\frac{dJ}{du_1} \mathrel{+}= \frac{dJ}{du}\frac{du}{du_1}, \quad \frac{du}{du_1} = 1 \qquad \frac{dJ}{du_2} \mathrel{+}= \frac{dJ}{du}\frac{du}{du_2}, \quad \frac{du}{du_2} = 1$
$u_1 = sin(t)$	$\frac{dJ}{dt} \mathrel{+}= \frac{dJ}{du_1}\frac{du_1}{dt}, \quad \frac{du_1}{dt} = \cos(t)$
$u_2 = 3t$	$\frac{dJ}{dt} \mathrel{+}= \frac{dJ}{du_2}\frac{du_2}{dt}, \quad \frac{du_2}{dt} = 3$
$t = x^2$	$\frac{dJ}{dx} \mathrel{+}= \frac{dJ}{dt}\frac{dt}{dx}, \quad \frac{dt}{dx} = 2x$

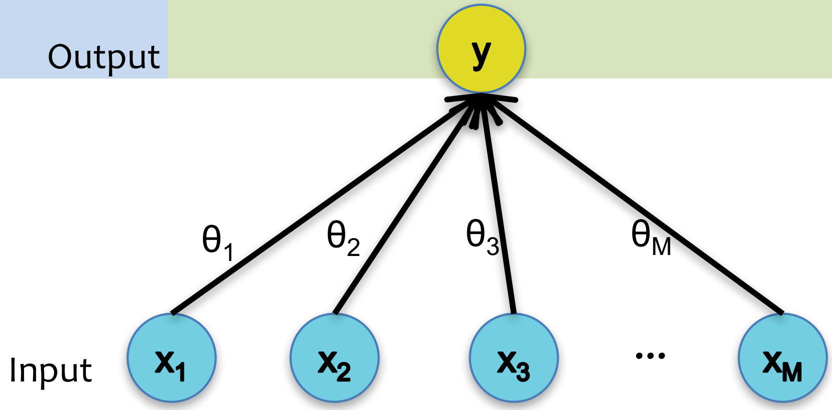
Training

Backpropagation

Whiteboard

- SGD for Neural Network
- Example: Backpropagation for Neural Network

Training Backpropagation



Case 1: Logistic Regression

Forward

$$J = y^* \log y + (1 - y^*) \log(1 - y)$$

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

$$a = \sum_{j=0}^{D} \theta_j x_j$$

Backward

$$\frac{dJ}{dy} = \frac{y^*}{y} + \frac{(1 - y^*)}{y - 1}$$

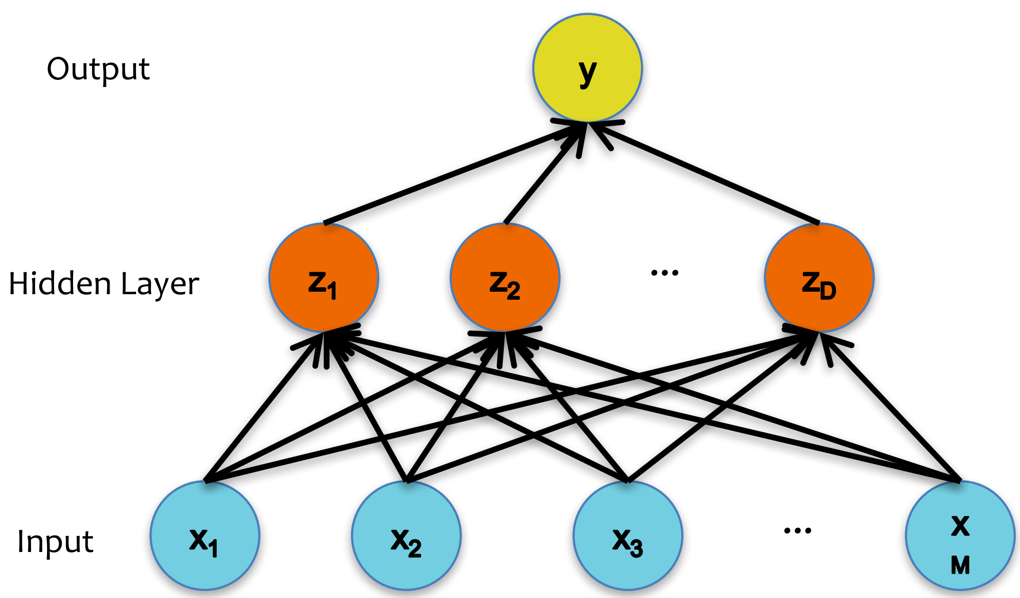
$$\frac{dJ}{da} = \frac{dJ}{dy}\frac{dy}{da}, \quad \frac{dy}{da} = \frac{\exp(-a)}{(\exp(-a) + 1)^2}$$

$$\frac{dJ}{d\theta_j} = \frac{dJ}{da}\frac{da}{d\theta_j}, \quad \frac{da}{d\theta_j} = x_j$$

$$\frac{dJ}{dx_j} = \frac{dJ}{da}\frac{da}{dx_j}, \quad \frac{da}{dx_j} = \theta_j$$

Training

Backpropagation



(E) **Output (sigmoid)**

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

(D) **Output (linear)**

$b = \sum_{j=0}^{D} \beta_j z_j$

(C) **Hidden (sigmoid)**

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

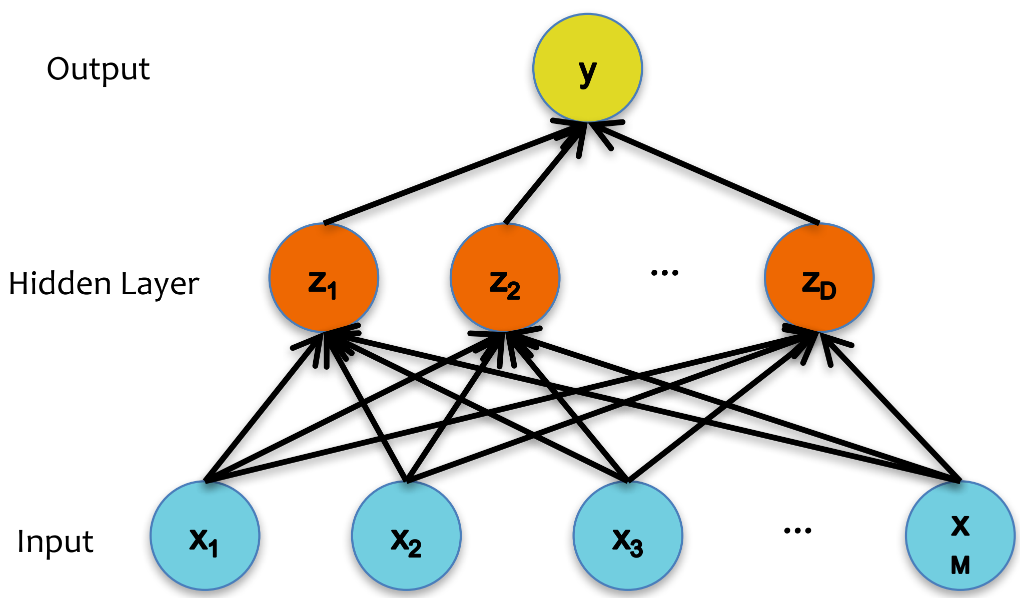
(B) **Hidden (linear)**

$a_j = \sum_{i=0}^{M} \alpha_{ji} x_i, \quad \forall j$

(A) **Input**

Given $x_i, \quad \forall i$

Training — Backpropagation



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

↑

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

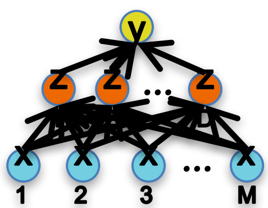
↑

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

Training

Backpropagation

Case 2: Neural Network



Forward

$$J = y^* \log y + (1 - y^*) \log(1 - y)$$

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

$$b = \sum_{j=0}^{D} \beta_j z_j$$

$$z_j = \frac{1}{1 + \exp(-a_j)}$$

$$a_j = \sum_{i=0}^{M} \alpha_{ji} x_i$$

Backward

$$\frac{dJ}{dy} = \frac{y^*}{y} + \frac{(1 - y^*)}{y - 1}$$

$$\frac{dJ}{db} = \frac{dJ}{dy}\frac{dy}{db}, \quad \frac{dy}{db} = \frac{\exp(-b)}{(\exp(-b) + 1)^2}$$

$$\frac{dJ}{d\beta_j} = \frac{dJ}{db}\frac{db}{d\beta_j}, \quad \frac{db}{d\beta_j} = z_j$$

$$\frac{dJ}{dz_j} = \frac{dJ}{db}\frac{db}{dz_j}, \quad \frac{db}{dz_j} = \beta_j$$

$$\frac{dJ}{da_j} = \frac{dJ}{dz_j}\frac{dz_j}{da_j}, \quad \frac{dz_j}{da_j} = \frac{\exp(-a_j)}{(\exp(-a_j) + 1)^2}$$

$$\frac{dJ}{d\alpha_{ji}} = \frac{dJ}{da_j}\frac{da_j}{d\alpha_{ji}}, \quad \frac{da_j}{d\alpha_{ji}} = x_i$$

$$\frac{dJ}{dx_i} = \frac{dJ}{da_j}\frac{da_j}{dx_i}, \quad \frac{da_j}{dx_i} = \sum_{j=0}^{D} \alpha_{ji}$$

Training

Backpropagation

Backpropagation (Auto.Diff. - Reverse Mode)

Forward Computation

1. Write an **algorithm** for evaluating the function $y = f(\mathbf{x})$. The algorithm defines a **directed acyclic graph**, where each variable is a node (i.e. the "**computation graph**")
2. Visit each node in **topological order**.
   a. Compute the corresponding variable's value
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Backward Computation

3. **Initialize** all partial derivatives dy/du_j to 0 and $dy/dy = 1$.
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   For variable $u_i = g_i(v_1,\dots, v_N)$
   a. We already know dy/du_i
   b. Increment dy/dv_j by $(dy/du_i)(du_i/dv_j)$
      (Choice of algorithm ensures computing (du_i/dv_j) is easy)

Return partial derivatives dy/du_i for all variables

Training Backpropagation

Case 2:

	Forward	Backward
Module 5	$J = y^* \log y + (1 - y^*) \log(1 - y)$	$\frac{dJ}{dy} = \frac{y^*}{y} + \frac{(1 - y^*)}{y - 1}$
Module 4	$y = \frac{1}{1 + \exp(-b)}$	$\frac{dJ}{db} = \frac{dJ}{dy}\frac{dy}{db}, \quad \frac{dy}{db} = \frac{\exp(-b)}{(\exp(-b) + 1)^2}$
Module 3	$b = \sum_{j=0}^{D} \beta_j z_j$	$\frac{dJ}{d\beta_j} = \frac{dJ}{db}\frac{db}{d\beta_j}, \quad \frac{db}{d\beta_j} = z_j$ $\frac{dJ}{dz_j} = \frac{dJ}{db}\frac{db}{dz_j}, \quad \frac{db}{dz_j} = \beta_j$
Module 2	$z_j = \frac{1}{1 + \exp(-a_j)}$	$\frac{dJ}{da_j} = \frac{dJ}{dz_j}\frac{dz_j}{da_j}, \quad \frac{dz_j}{da_j} = \frac{\exp(-a_j)}{(\exp(-a_j) + 1)^2}$
Module 1	$a_j = \sum_{i=0}^{M} \alpha_{ji} x_i$	$\frac{dJ}{d\alpha_{ji}} = \frac{dJ}{da_j}\frac{da_j}{d\alpha_{ji}}, \quad \frac{da_j}{d\alpha_{ji}} = x_i$ $\frac{dJ}{dx_i} = \frac{dJ}{da_j}\frac{da_j}{dx_i}, \quad \frac{da_j}{dx_i} = \sum_{j=0}^{D} \alpha_{ji}$

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!

Background

A Recipe for

1. Given training dat

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

2. Choose each of t

– Decision functio

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

– Loss function

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

opposite the gradient)

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

Summary

1. **Neural Networks…**
   - provide a way of learning features
   - are highly nonlinear prediction functions
   - (can be) a highly parallel network of logistic regression classifiers
   - discover useful hidden representations of the input
2. **Backpropagation…**
   - provides an efficient way to compute gradients
   - is a special case of reverse-mode automatic differentiation