DSC 140B
Representation Learning

Lecture 13 | Part 1

Neural Networks

Beyond RBFs

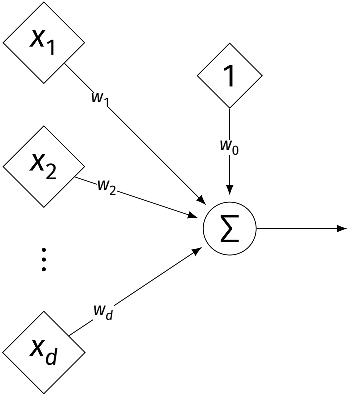
- When training RBFs, we fixed the basis functions *before* training the weights.

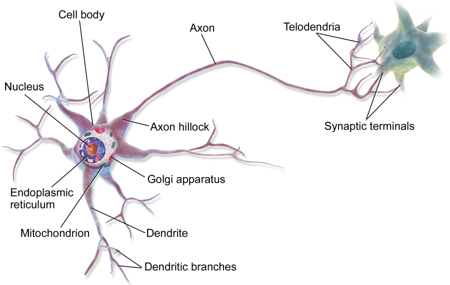
- Representation learning was decoupled from learning the prediction function.

- **Now:** learn representation **and** prediction function together.

Linear Models

$$H(\vec{x}) = w_0 + w_1 x_1 + \ldots + w_d x_d$$

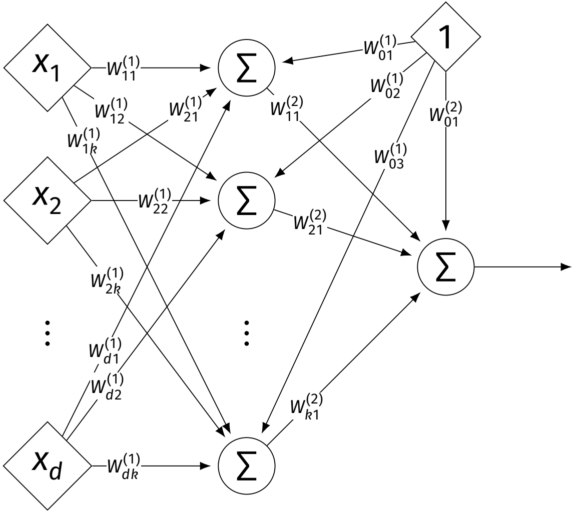




Generalizing Linear Models

- The brain is a **network** of neurons.
- The output of a neuron is used as an input to another.
- **Idea:** chain together multiple “neurons” into a **neural network**.

Neural Network[1] (One Hidden Layer)



[1]Specifically, a fully-connected, feed-forward neural network

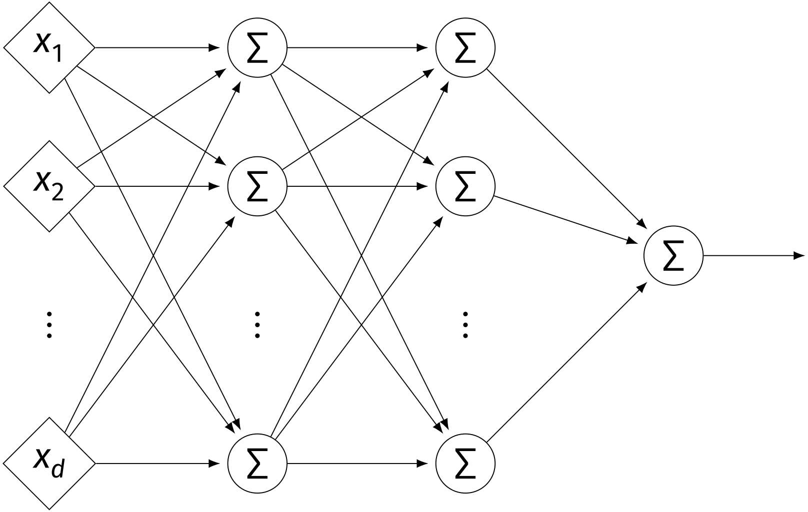
Architecture

- Neurons are organized into **layers**.
  - **Input layer**, **output layer**, and **hidden layers**.
- Number of cells in input layer determined by dimensionality of input feature vectors.
- Number of cells in hidden layer(s) is determined by you.
- Output layer can have >1 neuron.

Architecture

- Can have more than one hidden layer.
  - A network is “**deep**” if it has >1 hidden layer.
- Hidden layers can have different number of neurons.

Neural Network (Two Hidden Layers)

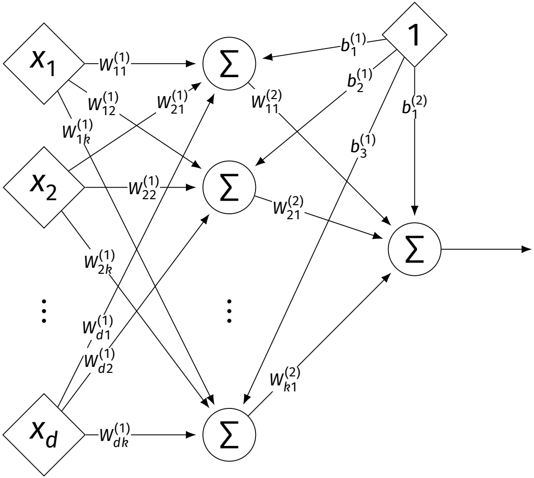


Network Weights

- A neural network is a type of function.
- Like a linear model, a NN is **totally determined** by its weights.
- But there are often many more weights to learn!

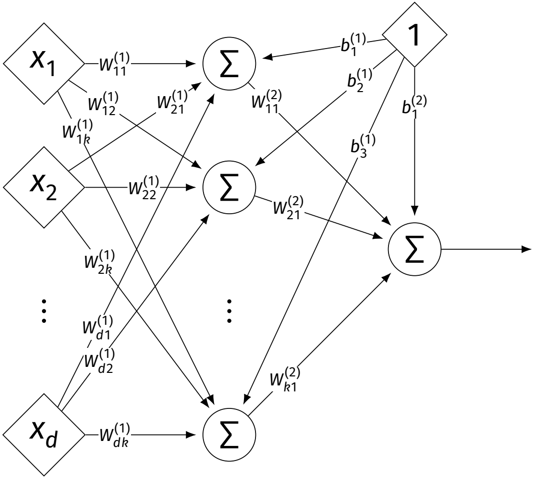
Notation

- Input is layer #0.
- $W^{(i)}_{jk}$ denotes weight of connection between neuron j in layer $(i-1)$ and neuron k in layer i
- Layer weights are 2-d arrays.



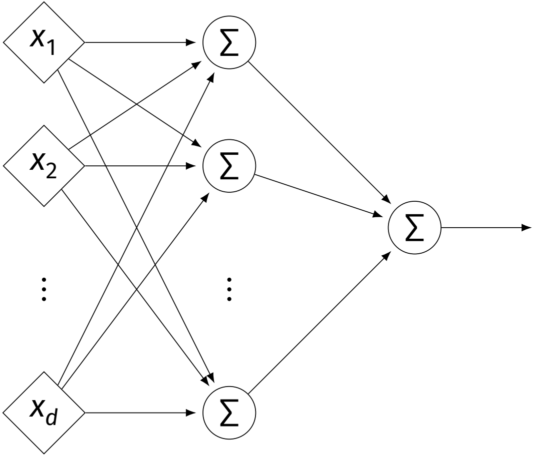
Notation

- Each hidden/output neuron gets a "dummy" input of 1.
- jth node in ith layer assigned a bias weight of $b_j^{(i)}$
- Biases for layer are a vector: $\vec{b}^{(i)}$

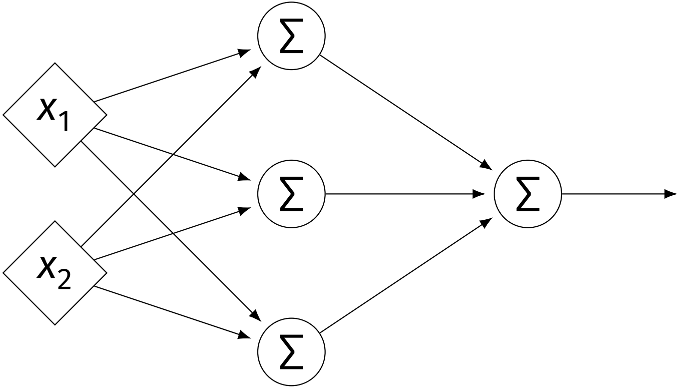


Notation

- Typically, we will not draw the weights.
- We will not draw the dummy input, too, but it is there.



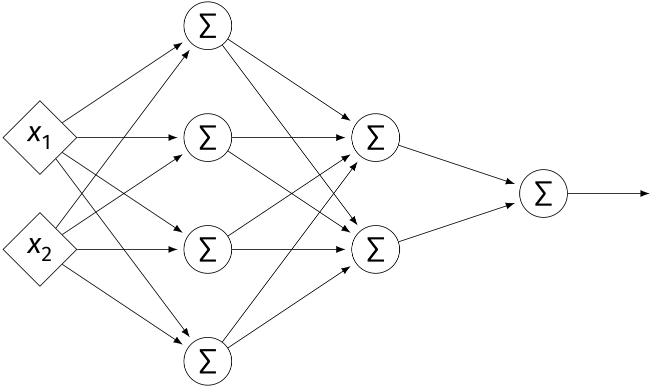
Example



$$W^{(1)} = \begin{pmatrix} 2 & -1 & 0 \\ 4 & 5 & 2 \end{pmatrix} \quad W^{(2)} = \begin{pmatrix} 3 \\ 2 \\ -4 \end{pmatrix}$$

$$\vec{b}^{(1)} = (3, -2, -2)^T \quad \vec{b}^{(2)} = (-4)^T$$

Example



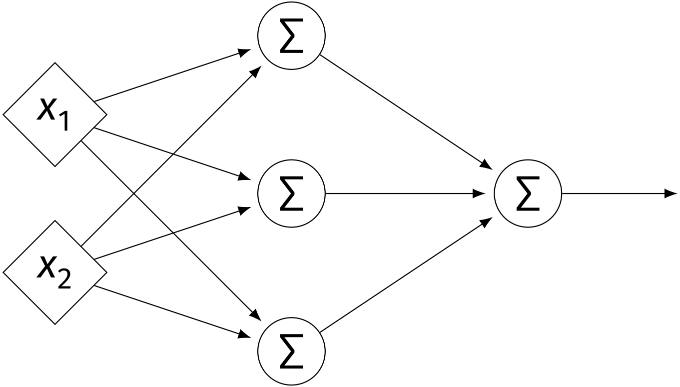
$$W^{(1)} = \begin{pmatrix} 2 & -1 & -3 & 0 \\ 4 & 5 & -7 & 2 \end{pmatrix} \quad W^{(2)} = \begin{pmatrix} 1 & 2 \\ -4 & 3 \\ -6 & -2 \\ 3 & 4 \end{pmatrix} \quad W^{(3)} = \begin{pmatrix} -1 & 5 \end{pmatrix}$$

$$\vec{b}^{(1)} = (3, 6, -2, -2)^T \quad \vec{b}^{(2)} = (-4, 0)^T \quad \vec{b}^{(3)} = (1)^T$$

Evaluation

- These are "**fully-connected, feed-forward**" networks with one output.
- They are functions $H(\vec{x}) : \mathbb{R}^d \to \mathbb{R}^1$
- To evaluate $H(\vec{x})$, compute result of layer i, use as inputs for layer $i + 1$.

Example



- $\vec{x} = (3, -1)^T$
- $z_1^{(1)} =$
- $z_2^{(1)} =$
- $z_3^{(1)} =$
- $z_1^{(2)} =$

$W^{(1)} = \begin{pmatrix} 2 & -1 & 0 \\ 4 & 5 & 2 \end{pmatrix}$ $W^{(2)} = \begin{pmatrix} 3 \\ 2 \\ -4 \end{pmatrix}$ $\vec{b}^{(1)} = (3, -2, -2)^T$ $\vec{b}^{(2)} = (-4)^T$

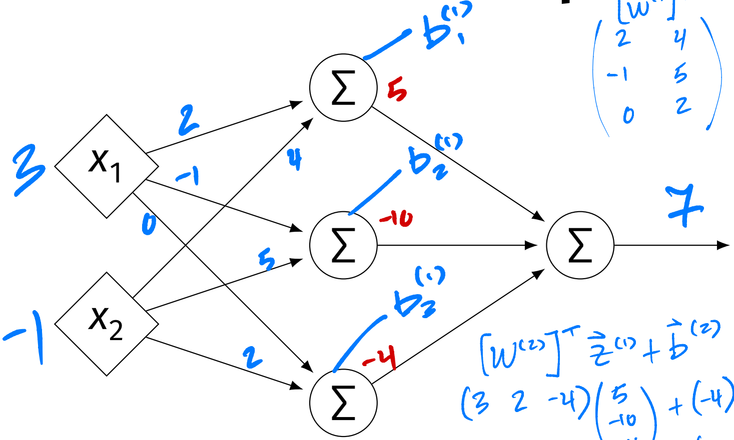
Evaluation as Matrix Multiplication

- Let $z_j^{(i)}$ be the output of node j in layer i.
- Make a vector of these outputs: $\vec{z}^{(i)} = (z_1^{(i)}, z_2^{(i)}, \ldots)^T$
- Observe that $\vec{z}^{(i)} = \left[W^{(i)}\right]^T \vec{z}^{(i-1)} + \vec{b}^{(i)}$

Example

$W^{(1)}\vec{x} + \vec{b}^{(1)}$

$$\underbrace{\begin{pmatrix}2 & 4\\ -1 & 5\\ 0 & 2\end{pmatrix}}_{[W^{(1)}]^T}\underbrace{\begin{pmatrix}3\\ -1\end{pmatrix}}_{\vec{x}} + \underbrace{\begin{pmatrix}3\\ -2\\ -2\end{pmatrix}}_{\vec{b}^{(1)}} = \begin{pmatrix}2\\ -8\\ -2\end{pmatrix} + \begin{pmatrix}3\\ -2\\ -2\end{pmatrix} = \begin{pmatrix}5\\ -10\\ -4\end{pmatrix}$$



- $\vec{x} = (3, -1)^T$
- $z_1^{(1)} = 5$
- $z_2^{(1)} = -10$
- $z_3^{(1)} = -4$
- $z_1^{(2)} = 7$

$[W^{(2)}]^T \vec{z}^{(1)} + \vec{b}^{(2)}$

$$\begin{pmatrix}3 & 2 & -4\end{pmatrix}\begin{pmatrix}5\\ -10\\ -4\end{pmatrix} + (-4) = (15 - 20 + 16 - 4) = 7$$

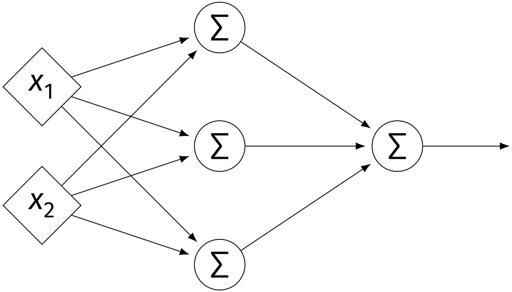
$W^{(1)} = \begin{pmatrix}2 & -1 & 0\\ 4 & 5 & 2\end{pmatrix}$ $W^{(2)} = \begin{pmatrix}3\\ 2\\ -4\end{pmatrix}$ $\vec{b}^{(1)} = (3, -2, -2)^T$ $\vec{b}^{(2)} = (-4)^T$

Each Layer is a Function

- We can think of each layer as a function mapping a vector to a vector.

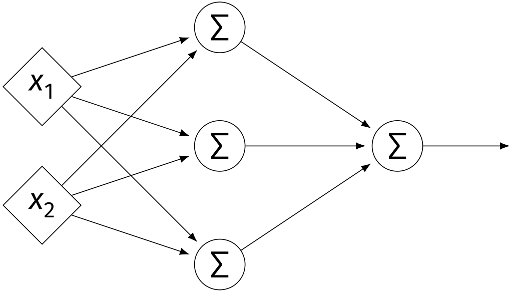
- $H^{(1)}(\vec{z}) = \left[W^{(1)}\right]^T \vec{z} + \vec{b}^{(1)}$
  - $H^{(1)} : \mathbb{R}^2 \to \mathbb{R}^3$

- $H^{(2)}(\vec{z}) = \left[W^{(2)}\right]^T \vec{z} + \vec{b}^{(2)}$
  - $H^{(2)} : \mathbb{R}^3 \to \mathbb{R}^1$



NNs as Function Composition

- The full NN is a composition of layer functions.



$$H(\vec{x}) = H^{(2)}(H^{(1)}(\vec{x})) = \left[W^{(2)}\right]^T \underbrace{\left(\left[W^{(1)}\right]^T \vec{x} + \vec{b}^{(1)}\right)}_{\vec{z}^{(1)}} + \vec{b}^{(2)}$$

NNs as Function Composition

- In general, if there k hidden layers:

$$H(\vec{x}) = H^{(k+1)}\left(\cdots H^{(3)}\left(H^{(2)}\left(H^{(1)}(\vec{x})\right)\right)\cdots\right)$$

Exercise

Show that:

$$H(\vec{x}) = \left[W^{(2)}\right]^T \left(\left[W^{(1)}\right]^T \vec{x} + \vec{b}^{(1)}\right) + \vec{b}^{(2)} = \vec{w} \cdot \text{Aug}(\vec{x})$$

for some appropriately-defined vector $\vec{w}$.

Result

- The composition of linear functions is again a linear function.
- The NNs we have seen so far are all equivalent to linear models!
- For NNs to be more useful, we will need to add **non-linearity**.

Activations

- So far, the output of a neuron has been a linear function of its inputs:

$$w_0 + w_1 x_1 + w_2 x_2 + \ldots$$

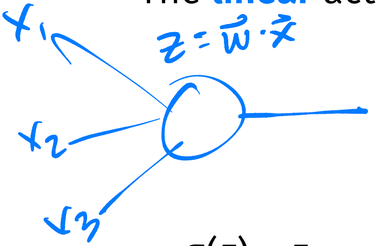
- Can be arbitrarily large or small.
- But real neurons are **activated** non-linearly.
  - E.g., saturation.

Idea

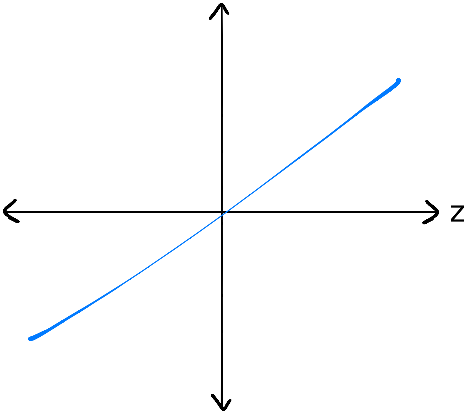
- To add nonlinearity, we will apply a non-linear **activation function** g to the output of **each** hidden neuron (and sometimes the output neuron).

Linear Activation

- The **linear** activation is what we've been using.

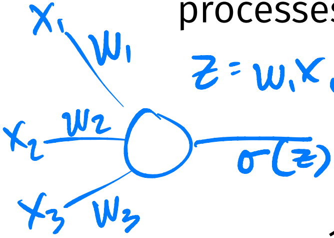


$$\sigma(z) = z$$

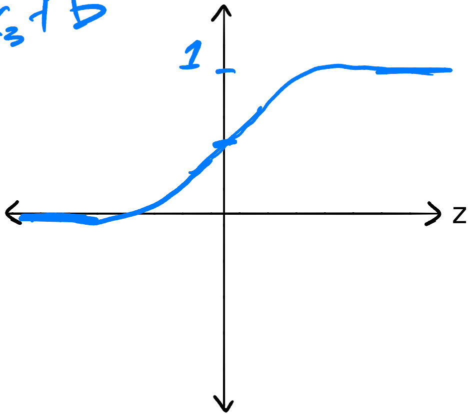


Sigmoid Activation

- The **sigmoid** models saturation in many natural processes.



$$z = w_1x_1 + w_2x_2 + w_3x_3 + b$$



$$\sigma(z) = \frac{1}{1 + e^{-z}}$$

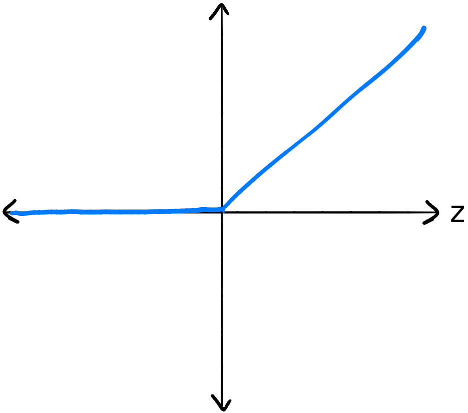
$\sigma(-\infty) = 0$ $\quad\quad$ $\sigma(0) = \frac{1}{2}$

$\sigma(\infty) = 1$

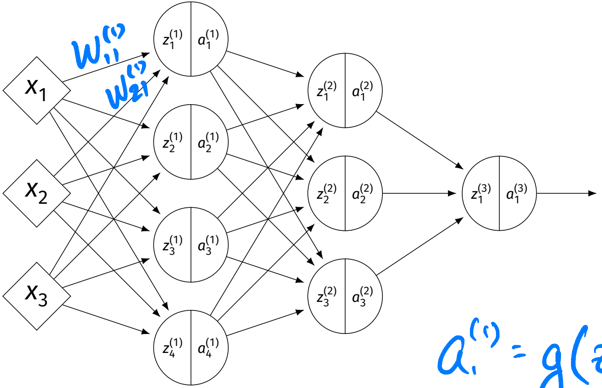
ReLU Activation

- The **Rectified Linear Unit (ReLU)** tends to work better in practice.

$$g(z) = \max\{0, z\}$$



Notation



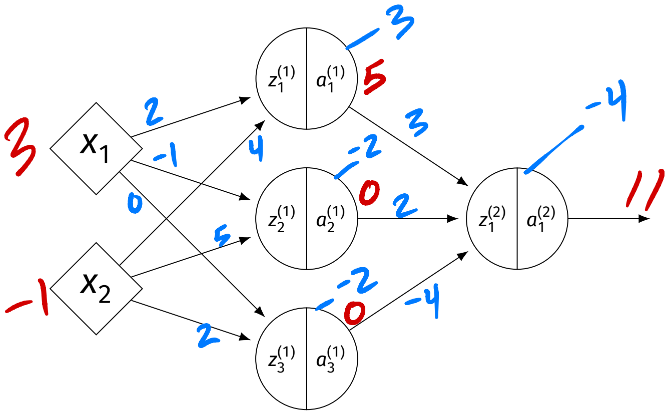
$$z_1^{(1)} = w_{11}^{(1)} x_1 + w_{21}^{(1)} x_2 + w_{31}^{(1)} x_3 + b_1^{(1)}$$

$$a_1^{(1)} = g(z_1^{(1)})$$

- $z_j^{(i)}$ is the linear activation before g is applied.
- $a_j^{(i)} = g(z^{(i)})$ is the actual output of the neuron.

Example

$(2)(3) + (4)(-1) + 3$
$= 6 - 4 + 3 = 5$



- g = ReLU
- Linear output
- $\vec{x} = (3, -1)^T$
- $z_1^{(1)} = 5$
- $a_1^{(1)} = g(5) = 5$
- $z_2^{(1)} = 0 \quad -10$
- $a_2^{(1)} = g(-10) = 0$
- $z_3^{(1)} = -4$
- $a_3^{(1)} = g(-4) = 0$
- $z_1^{(2)} = 11$

$a_1^{(2)} = 11$

$W^{(1)} = \begin{pmatrix} 2 & -1 & 0 \\ 4 & 5 & 2 \end{pmatrix}$ $\quad W^{(2)} = \begin{pmatrix} 3 \\ 2 \\ -4 \end{pmatrix}$ $\quad \vec{b}^{(1)} = (3, -2, -2)^T$ $\quad \vec{b}^{(2)} = (-4)^T$

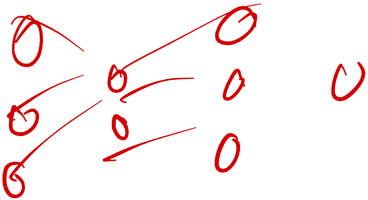
$$\vec{z}^{(\ell)} = g\left(W^{(\ell)} \vec{z}^{(\ell-1)} + \vec{b}^{(\ell)}\right)$$

Output Activations

- The activation of the output neuron(s) can be different than the activation of the hidden neurons.
- In classification, **sigmoid** activation makes sense.
- In regression, **linear** activation makes sense.

Main Idea

A neural network with linear activations is a linear model. If non-linear activations are used, the model is made non-linear.



DSC 140B

Representation Learning

Lecture 13 | Part 2

Demo

Feature Map

- We have seen how to fit non-linear patterns with linear models via **basis functions** (i.e., a feature map).

$$H(\vec{x}) = w_0 + w_1\phi_1(\vec{x}) + \ldots + w_k\phi_k(\vec{x})$$

- These basis functions are fixed **before** learning.
- **Downside:** we have to choose $\vec{\phi}$ somehow.

Learning a Feature Map

- **Interpretation:** The hidden layers of a neural network **learn** a feature map.

Each Layer is a Function

- We can think of each layer as a function mapping a vector to a vector.

- $H^{(1)}(\vec{z}) = \left[W^{(1)}\right]^T \vec{z} + \vec{b}^{(1)}$
  - $H^{(1)} : \mathbb{R}^2 \to \mathbb{R}^3$
- $H^{(2)}(\vec{z}) = \left[W^{(2)}\right]^T \vec{z} + \vec{b}^{(2)}$
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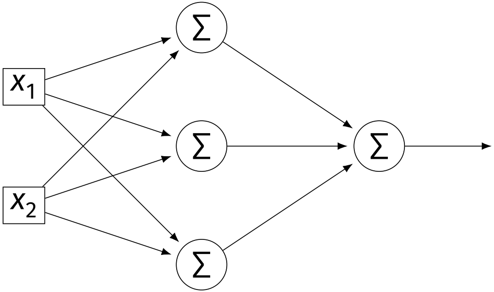
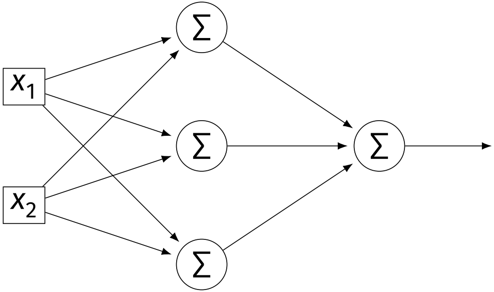


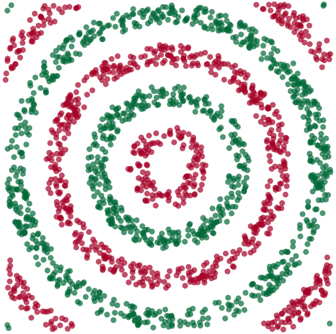
Each Layer is a Function

- The hidden layer performs a feature map from $\mathbb{R}^2$ to $\mathbb{R}^3$.
- The output layer makes a prediction in $\mathbb{R}^3$.
- **Intuition:** The feature map is learned so as to make the output layer's job "easier".



Demo

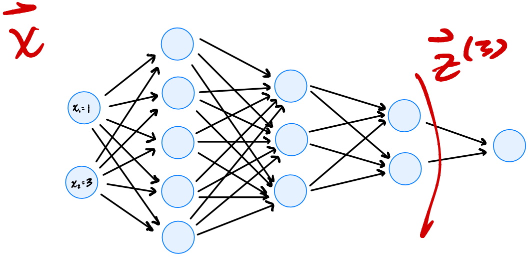
- Train a deep network to classify the data below.
- Hidden layers will learn a new feature map that makes the data linearly separable.



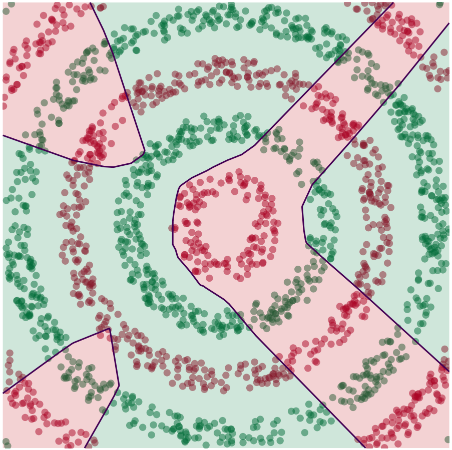
Demo

$\vec{x} \mapsto \vec{z}^{(3)}$

- We'll use three hidden layers, with last having two neurons.
- We can see this new representation!
- Plug in $\vec{x}$ and see activations of last hidden layer.



Learning a New Representation



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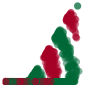

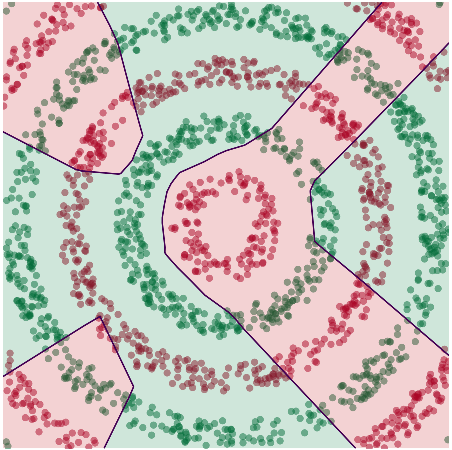

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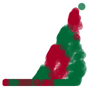
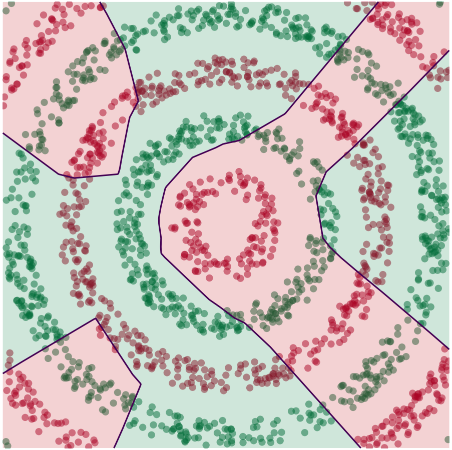
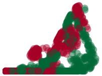
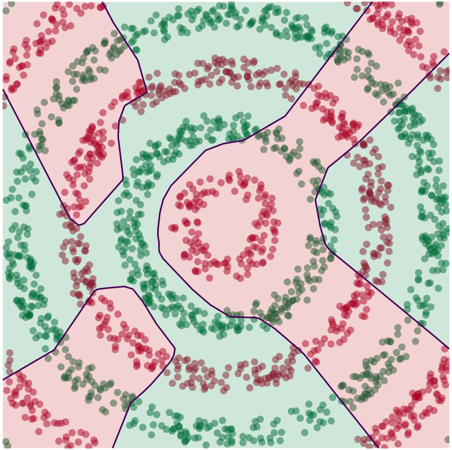


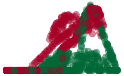


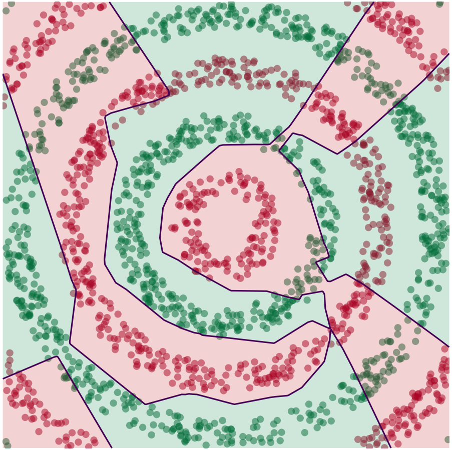
Learning a New Representation



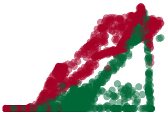


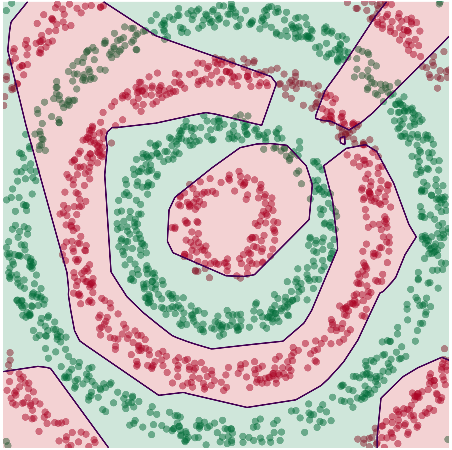
Learning a New Representation



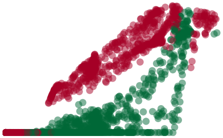


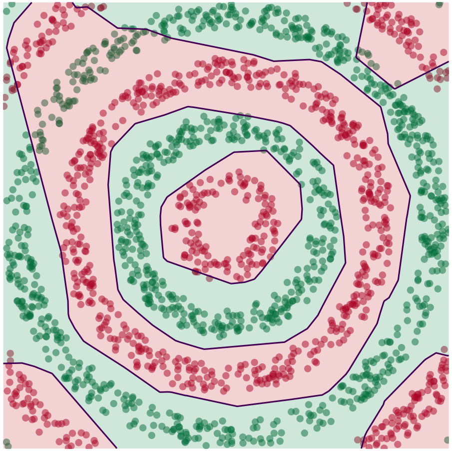
Learning a New Representation



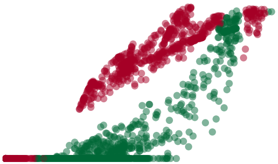


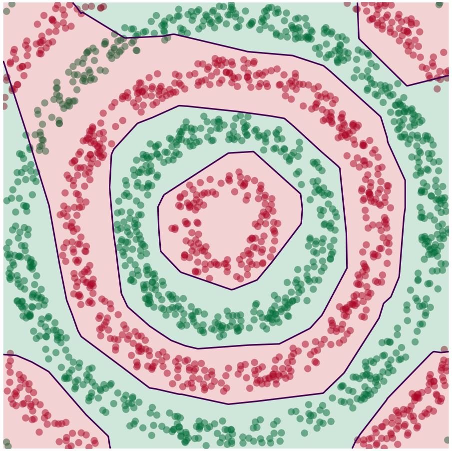
Learning a New Representation



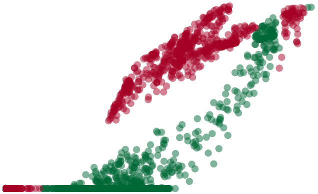


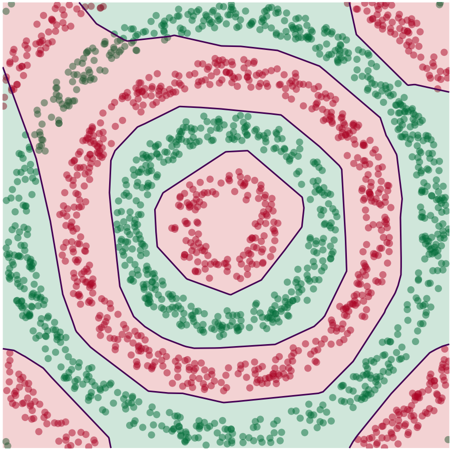
Learning a New Representation



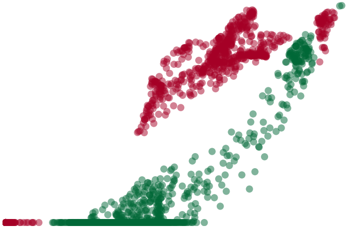


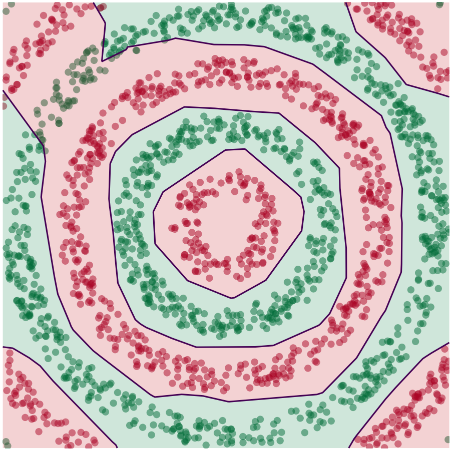
Learning a New Representation



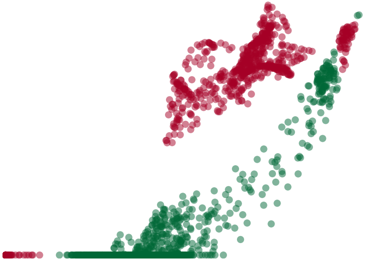


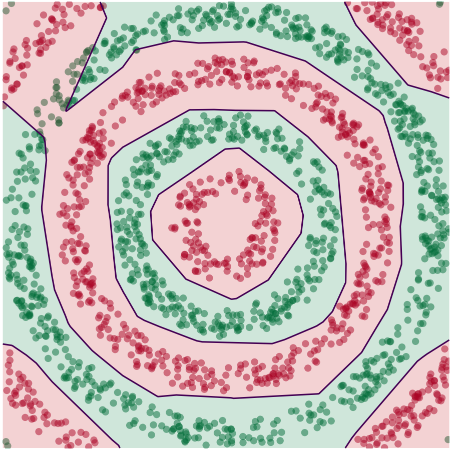
Learning a New Representation



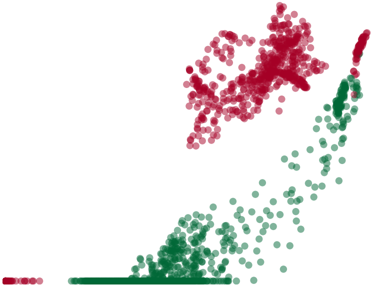


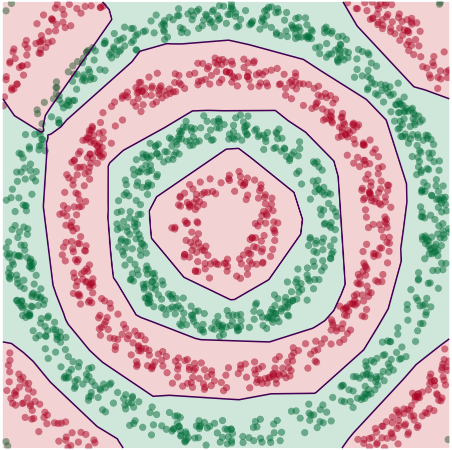
Learning a New Representation



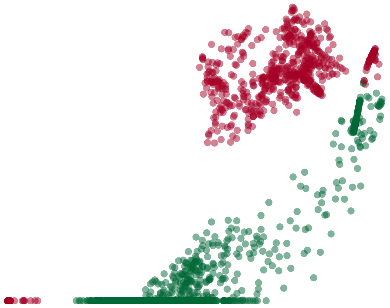


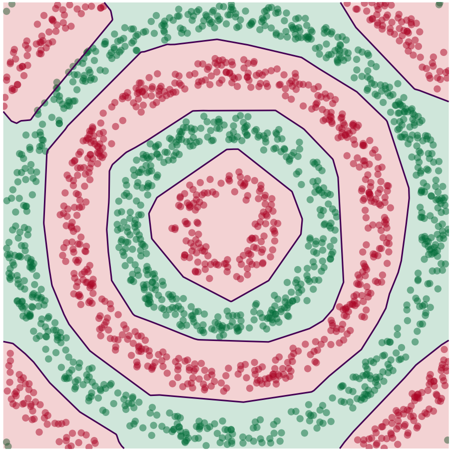
Learning a New Representation



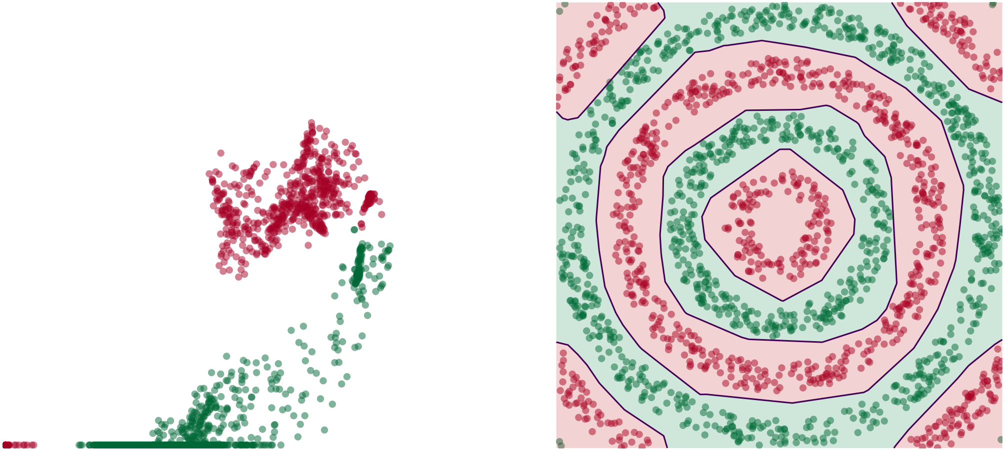


Learning a New Representation

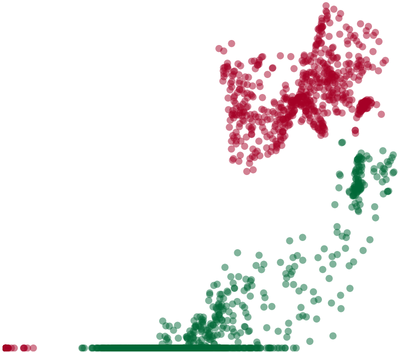


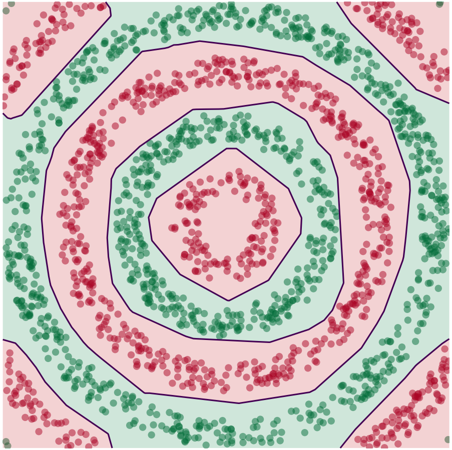


Learning a New Representation

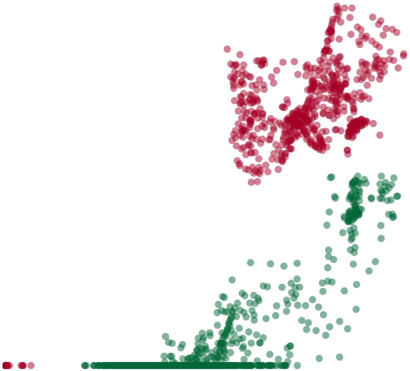


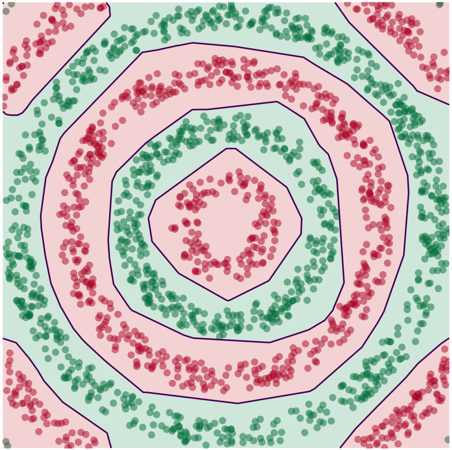
Learning a New Representation



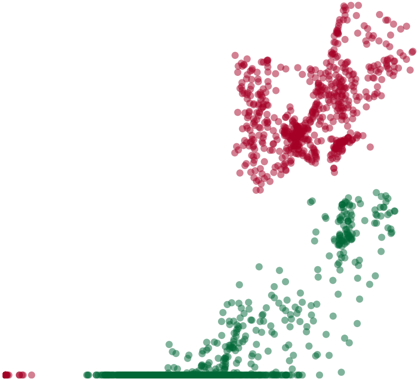


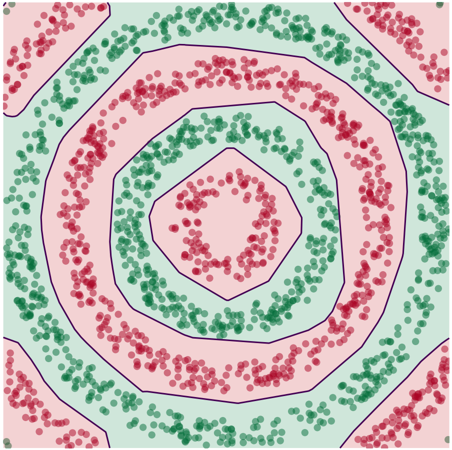
Learning a New Representation



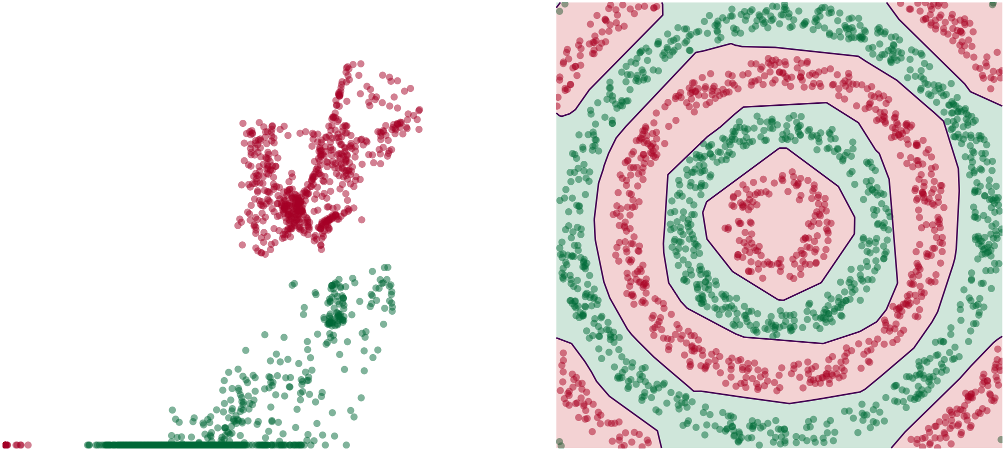


Learning a New Representation

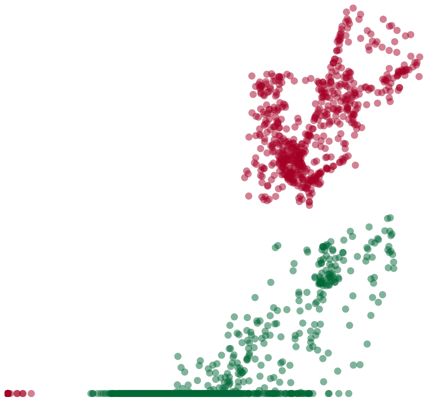


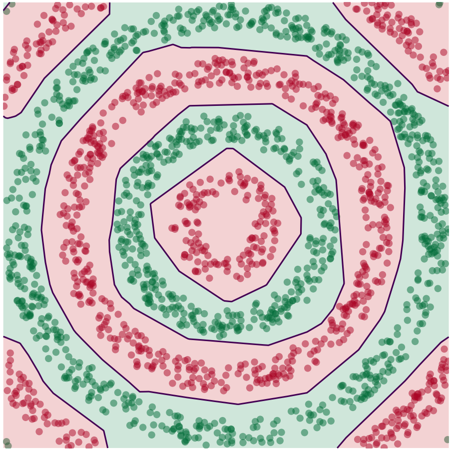


Learning a New Representation



Learning a New Representation





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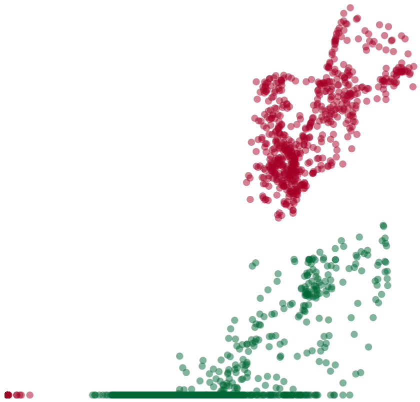

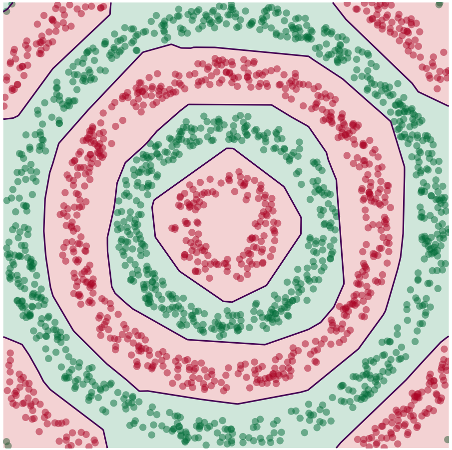

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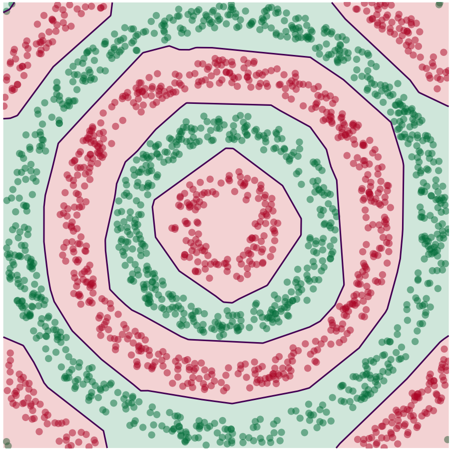

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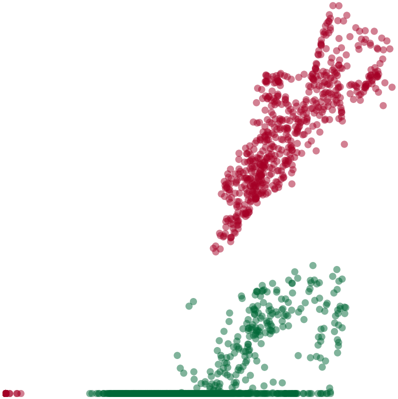
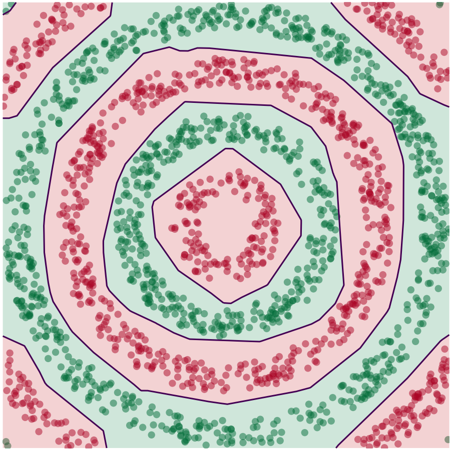
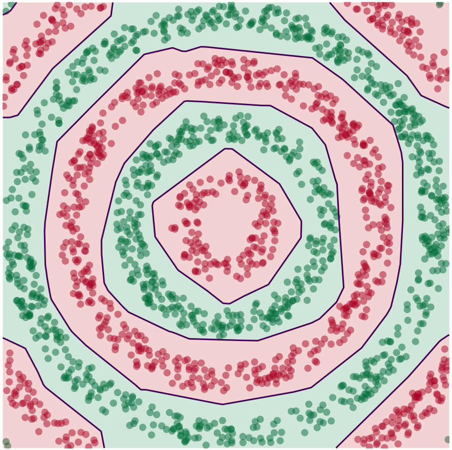
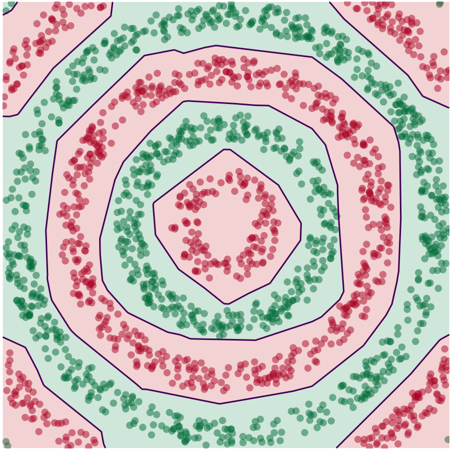




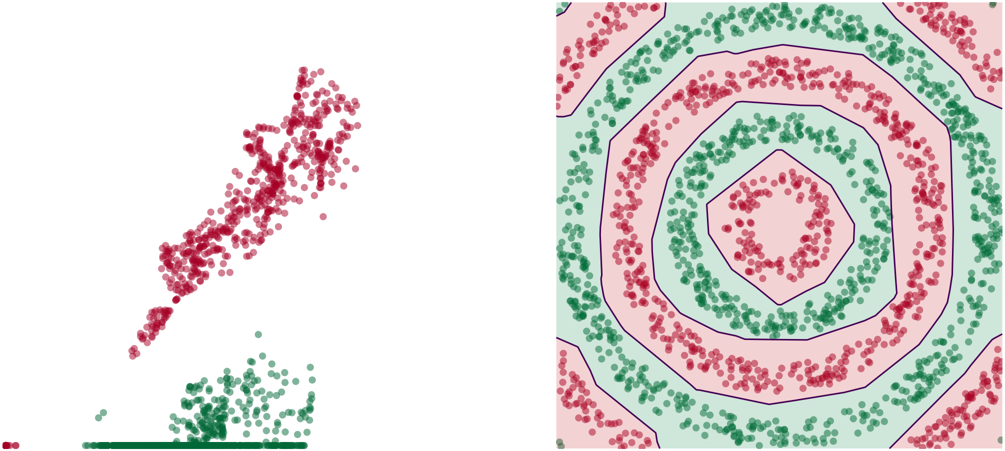
Learning a New Representation



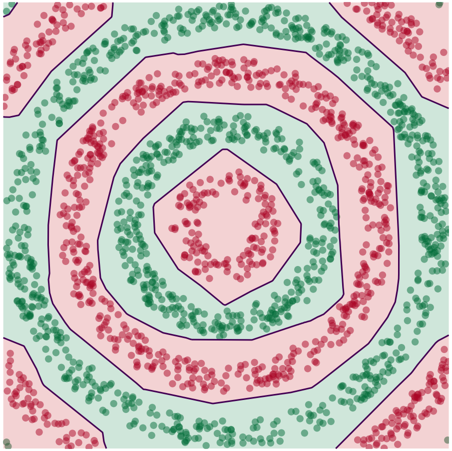
Learning a New Representation



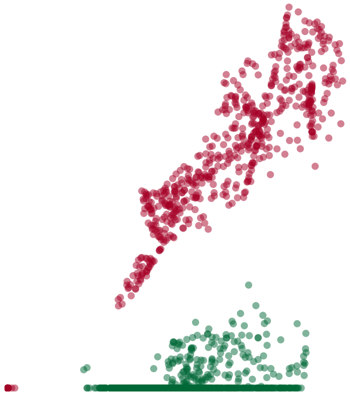
Learning a New Representation

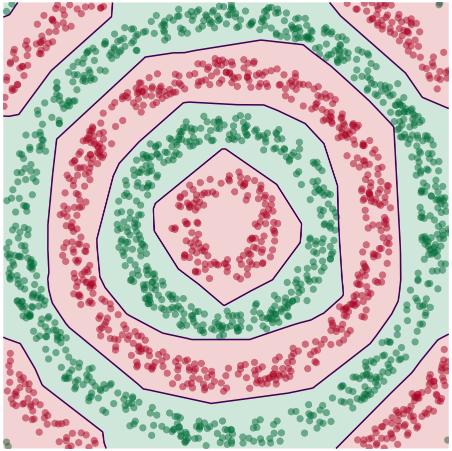


Learning a New Representation

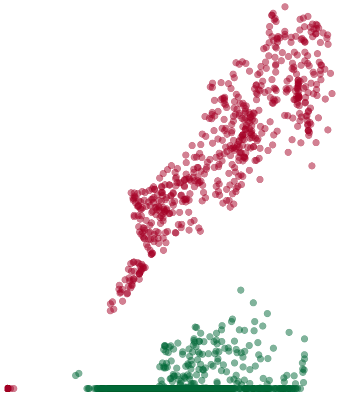


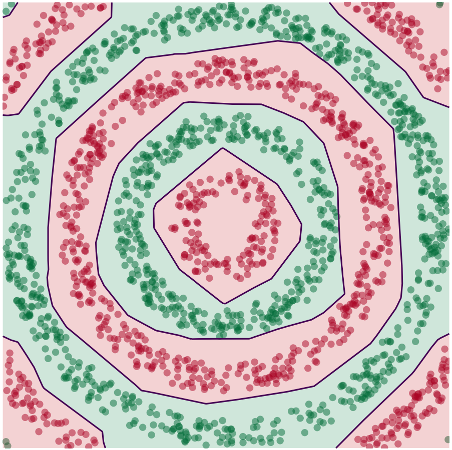
Learning a New Representation



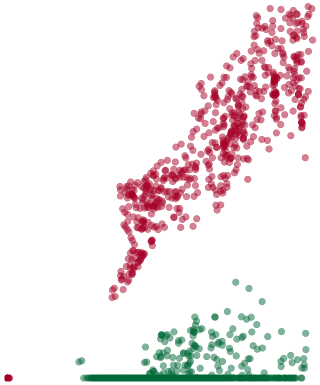


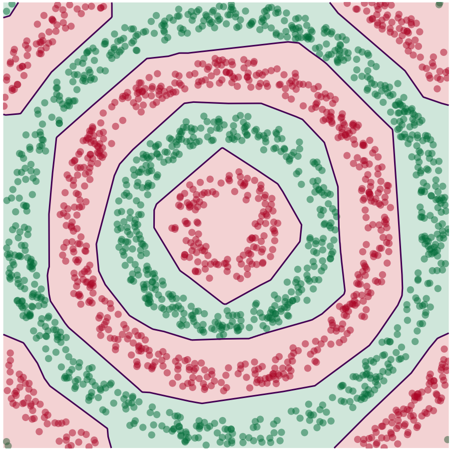
Learning a New Representation



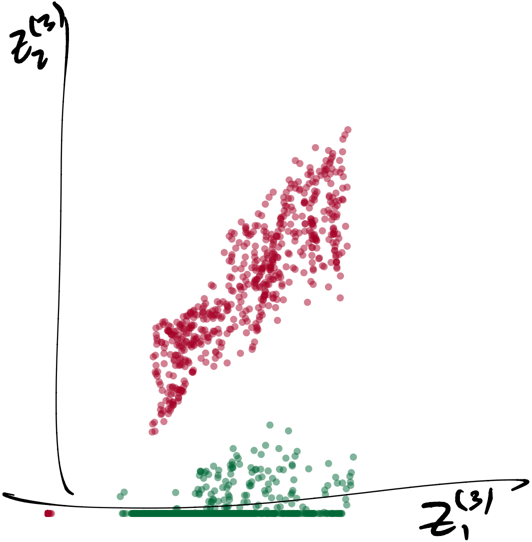


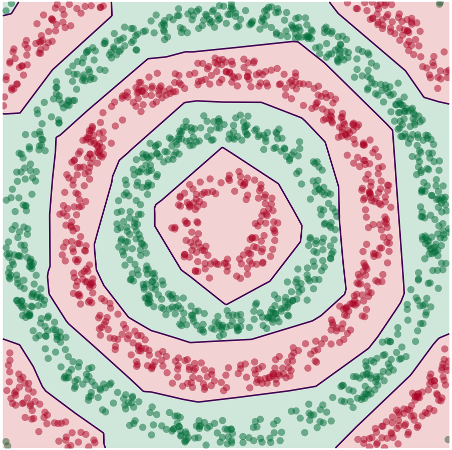
Learning a New Representation





Learning a New Representation





Deep Learning

- The NN has learned a new **representation** in which the data is easily classified.

DSC 140B

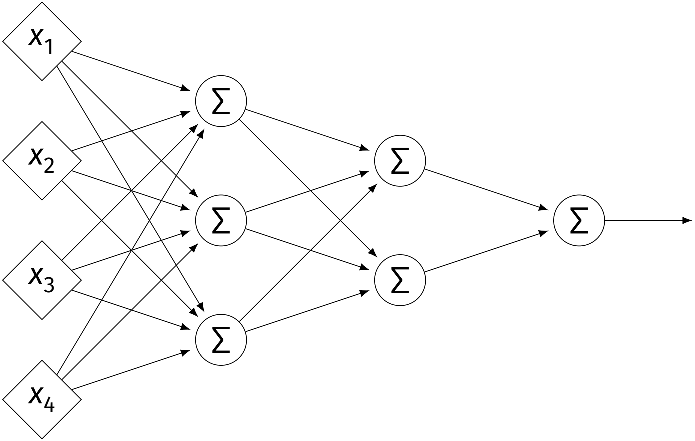
Representation Learning

Lecture 13 | Part 3

Training Neural Networks

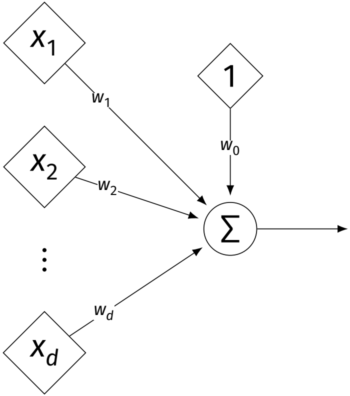
Training

- How do we learn the weights of a (deep) neural network?



Remember...

- How did we learn the weights in linear least squares regression?



Empirical Risk Minimization

0. Collect a training set, $\{(\vec{x}^{(i)}, y_i)\}$
1. Pick the form of the prediction function, H.
2. Pick a loss function.
3. Minimize the empirical risk w.r.t. that loss.

Remember: Linear Least Squares

0. Pick the form of the prediction function, H.
   - E.g., linear: $H(\vec{x};\vec{w}) = w_0 + w_1 x_1 + \ldots + w_d x_d = \text{Aug}(\vec{x}) \cdot \vec{w}$
1. Pick a loss function.
   - E.g., the square loss. $(H(\vec{x}^{(i)}) - y_i)^2$
2. Minimize the empirical risk w.r.t. that loss:

$$R_{\text{sq}}(\vec{w}) = \frac{1}{n}\sum_{i=1}^{n}(H(\vec{x}^{(i)}) - y_i)^2 = \frac{1}{n}\sum_{i=1}^{n}(\text{Aug}(\vec{x}^{(i)}) \cdot \vec{w} - y_i)^2$$

$$\frac{d}{dx} f(x) = 0$$

$$\vec{w} = (X^T X)^{-1} X^T \vec{y}$$

Minimizing Risk

- To minimize risk, we often use **vector calculus**.
  - Either set $\nabla_{\vec{w}} R(\vec{w}) = 0$ and solve...
  - Or use gradient descent: walk in opposite direction of $\nabla_{\vec{w}} R(\vec{w})$.

- Recall, $\nabla_{\vec{w}} R(\vec{w}) = (\partial R / \partial w_0, \partial R / \partial w_1, \ldots, \partial R / \partial w_d)^T$

$$\frac{d}{d\vec{w}} R(\vec{w}) = \nabla_{\vec{w}} R(\vec{w})$$

In General

- Let ℓ be the loss function, let $H(\vec{x};\vec{w})$ be the prediction function.

- The empirical risk:

$$R(\vec{w}) = \frac{1}{n}\sum_{i=1}^{n} \ell(H(\vec{x}^{(i)};\vec{w}), y_i)$$

- Using the chain rule:

$$\nabla_{\vec{w}} R(\vec{w}) = \frac{1}{n}\sum_{i=1}^{n} \frac{\partial \ell}{\partial H} \nabla_{\vec{w}} H(\vec{x}^{(i)};\vec{w})$$

Gradient of H

- To minimize risk, we want to compute $\nabla_{\vec{w}} R$.
- To compute $\nabla_{\vec{w}} R$, we want to compute $\nabla_{\vec{w}} H$.
- This will depend on the form of H.

Example: Linear Model

- Suppose H is a linear prediction function:

$$H(\vec{x}; \vec{w}) = w_0 + w_1 x_1 + \ldots + w_d x_d$$

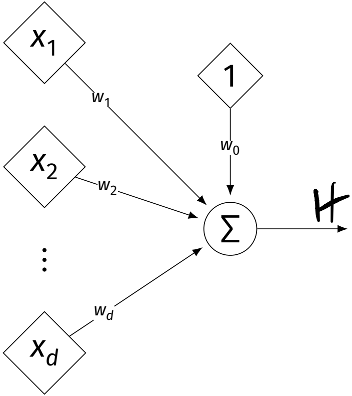
- What is $\nabla_{\vec{w}} H$ with respect to $\vec{w}$?

$$\nabla_{\vec{w}} H = \left(\frac{\partial H}{\partial w_0}, \frac{\partial H}{\partial w_1}, \ldots, \frac{\partial H}{\partial w_d} \right)^T$$

$$= (1, x_1, x_2, \ldots, x_d)^T$$

Example: Linear Model

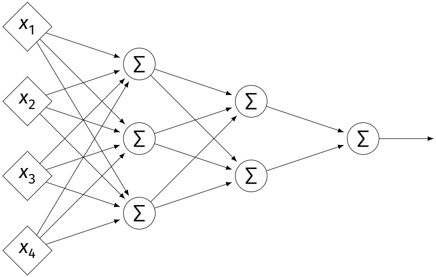
- Consider $\partial H / \partial w_1$: $= x_1$



Example: Neural Networks

- Suppose H is a neural network (with nonlinear activations).

- What is ∇H?
  - It's more complicated...



Parameter Vectors

- It is often useful to pack all of the network's weights into a **parameter vector**, $\vec{w}$.
- Order is arbitrary:

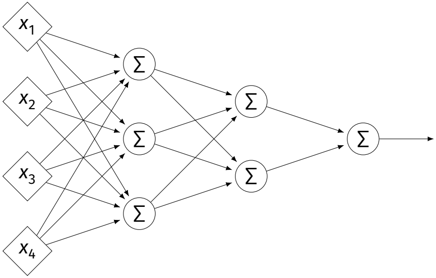
$$\vec{w} = (W_{11}^{(1)}, W_{12}^{(1)}, \ldots, b_1^{(1)}, b_2^{(1)}, W_{11}^{(2)}, W_{12}^{(2)}, \ldots, b_1^{(2)}, b_2^{(2)}, \ldots)^T$$

- The network is a function $H(\vec{x}; \vec{w})$.
- Goal of learning: find the "best" $\vec{w}$.

Example: Neural Networks

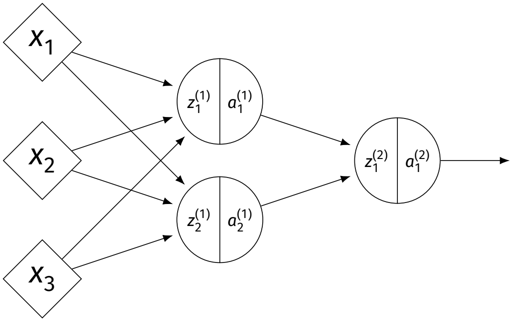
- $\nabla_{\vec{w}} H$ is a vector-valued function with one entry per parameter.

- Plugging a data point, $\vec{x}$, and a parameter vector, $\vec{w}$, into $\nabla_{\vec{w}} H$ "evaluates the gradient", results in a vector.



Exercise

Suppose $W_{11}^{(1)} = -2, W_{21}^{(1)} = -5, W_{31}^{(1)} = 2$ and $\vec{x} = (3, 2, -2)^T$ and all biases are 0. ReLU activations are used. What is $\partial H / \partial W_{11}^{(1)}(\vec{x}, \vec{w})$?



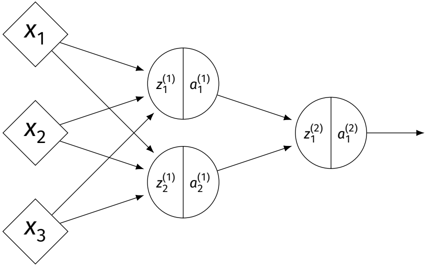
Recall: Chain Rule

$$\frac{df}{dx}[f(g(x))] = \frac{df}{dg}(g(x))\,\frac{dg}{dx}$$

$$= f'(g(x))\,g'(x)$$

Example: Neural Network

- Compute $\partial H / \partial W_{11}^{(1)}$ for the network shown below. Assume the hidden layer activation function is σ.

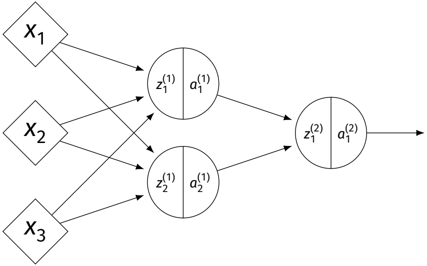


$$W^{(1)} = \begin{pmatrix} 3 & 2 \\ 4 & 1 \\ 1 & 3 \end{pmatrix} \quad W^{(2)} = \begin{pmatrix} 3 \\ 1 \end{pmatrix}$$

$$\vec{x} = (3, 1, 2)^T$$

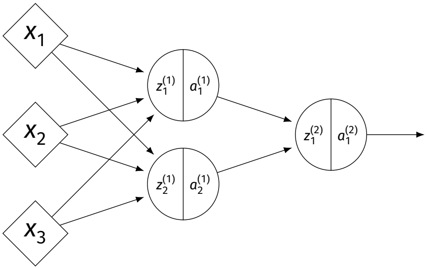
Example: Neural Network

- Compute $\partial H / \partial W_{11}^{(1)}$ for the network shown below. Assume the hidden layer activation function is σ.



Example: Neural Network

- Compute $\partial H / \partial W_{21}^{(1)}$ for the network shown below. Assume the hidden layer activation function is σ.

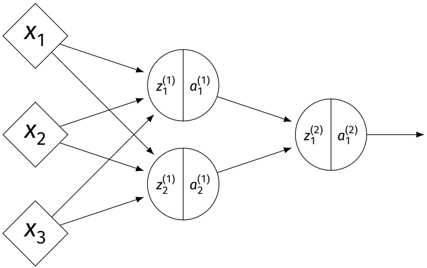


$$W^{(1)} = \begin{pmatrix} 3 & 2 \\ 4 & 1 \\ 1 & 3 \end{pmatrix} \quad W^{(2)} = \begin{pmatrix} 3 \\ 1 \end{pmatrix}$$

$$\vec{x} = (3, 1, 2)^T$$

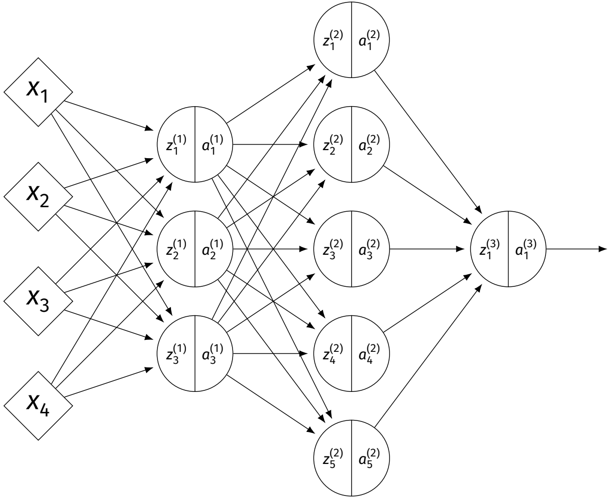
Example: Neural Network

- Compute $\partial H/\partial W^{(1)}_{21}$ for the network shown below. Assume the hidden layer activation function is σ.



Imagine...

- Compute $W_{11}^{(1)}$:



A Better Way

- Computing the gradient is straightforward…
- But can involve a lot of redundant work.
- **Backpropagation** is a methodical approach to computing the gradient that is more efficient.