

DSCI 572: Supervised Learning II

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Feedforward Neural Networks

Biological Inspiration

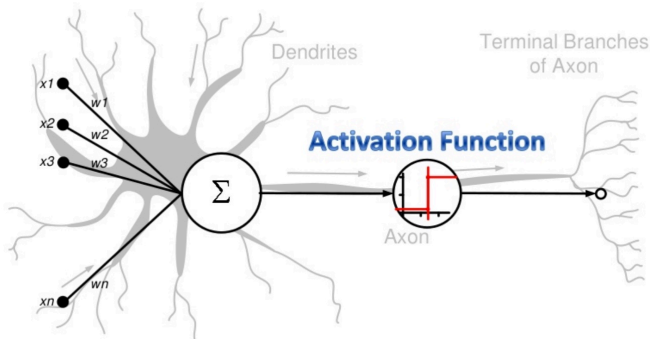


Figure: Information processing in the brain. **Weights** between neurons model whether they **excite** or **inhibit** one another. Activation can be viewed as **firing rates**. **Activation functions and bias** model the **thresholded behavior of action potentials**. (Recall: action potential is an electric impulse traveling through an axon when a neuron is excited above a threshold). [From Andrew Nelson]

Hubel and Wiesel Cat Experiment



Listen to Neurons

Hubel and Wiesel could listen to the neurons of a cat firing as they moved lines of light in certain directions before the retina of a cat's eye. Listen [here] and [here].

An Artificial Neuron



Figure: One neuron, with an activation function

Neuron With Input

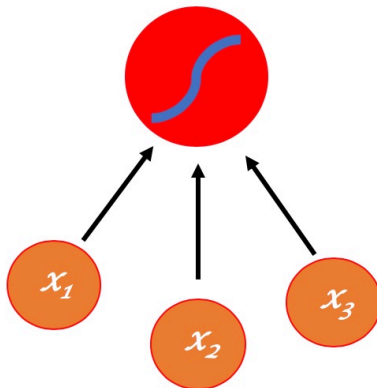


Figure: Input is a vector of \mathbf{x} with three units, each taking an index j

A Vector For Connection Weights

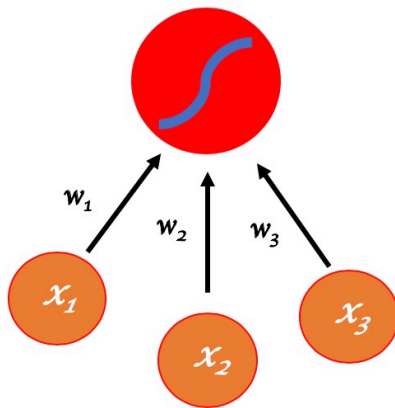


Figure: A vector of free parameters \mathbf{w} with several items, each taking an index i

A Bias Unit

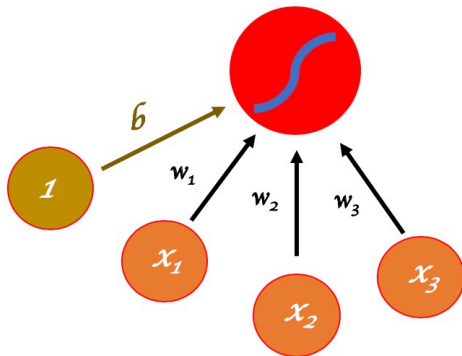


Figure: A bias unit b , equal to 1

A Deep Neural Network

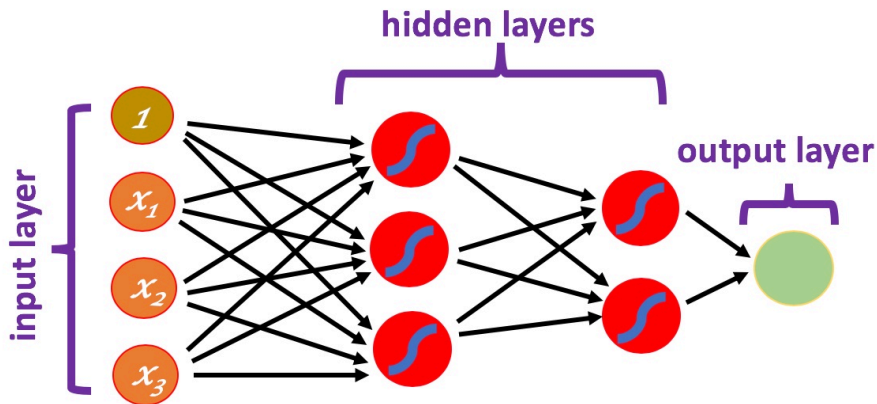


Figure: A **deep neural network**. The network has **2 hidden layers**.

What are Feedforward Nets?

- Also called **multilayer perceptrons (MLP)**.
- A **mapping function** of input x to a category y s.t. $y = f(x; \theta)$
- **Goal:** To learn the value of the parameters θ .
- It is a **directed acyclic graph**, e.g., $f(x) = f^{(3)}(f^{(2)}(f^{(1)}))$.
- Each of the three functions is one **layer**, in the **deep network**.
- **No feedback connections** in which outputs of the model are fed back into itself, otherwise the network would be a **recurrent neural network**.

Learning Good Representations

- We want to **identify a function** $\phi(x)$ that we use to acquire a new representation of x .
- $\phi(x)$ defines a **hidden layer**.
- In DL, we actually **learn this function** ϕ .
- We parametrize the representation as

$$\phi(x; \theta)$$

and use the **optimization algorithm** to find the θ that corresponds to a good representation.

- In DL, we use **gradient-based optimization**.

XOR Function

- The **XOR function** ("exclusive or") is an operation on two binary values, x_1 and x_2 .
- When *exactly one* of these binary values is equal to 1, the XOR function returns 1. Otherwise, it returns 0.

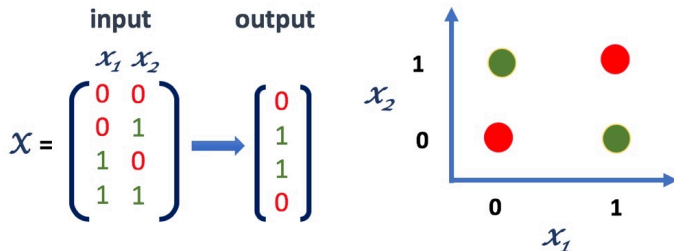


Figure: XOR Function

A Simple Feedforward Neural Network

a single hidden layer network

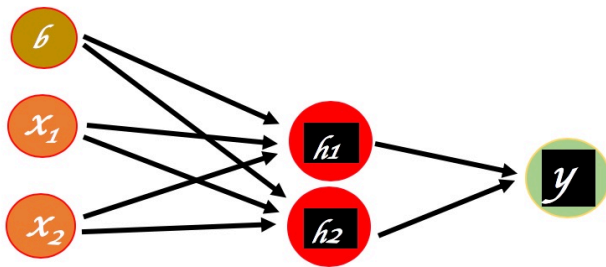


Figure: A simple feedforward network for solving XOR function. Connection weights from input to hidden will be a 2×2 matrix \mathbf{W} . We will refer to the matrix as $\mathbf{W}^{(1)}$ to denote it is the first layer matrix (input-to-hidden). Weights from hidden to output will be a vector $\mathbf{w}^{(2)}$ of 2 dimensions. We will also add bias.

A Feedforward Neural Network With Weights

the network with weights

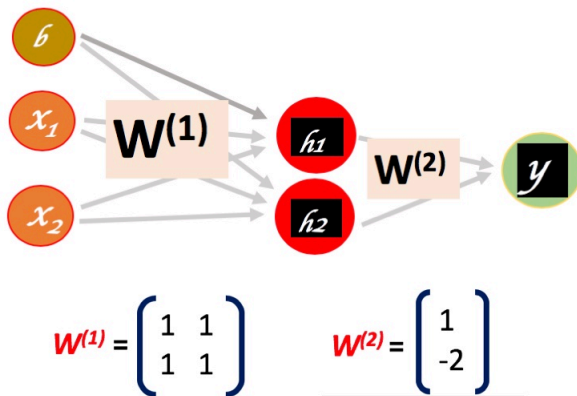


Figure: The network with weights. The hidden layer has one bias unit that is dropped from diagram, for simplicity.

Components of a Feedforward Network (For Solving XOR)

$$\begin{aligned} \mathbf{W} &= \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} & \mathbf{X} &= \begin{matrix} \mathbf{x}_1 & \mathbf{x}_2 \\ \begin{bmatrix} 0 & 0 \\ 0 & 1 \\ 1 & 0 \\ 1 & 1 \end{bmatrix} \end{matrix} \\ \mathbf{c} &= \begin{bmatrix} 0 \\ -1 \end{bmatrix} & \mathbf{b} &= \begin{bmatrix} 0 \end{bmatrix} \\ \mathbf{w} &= \begin{bmatrix} 1 \\ -2 \end{bmatrix} \end{aligned}$$

Figure: Ingredients of the Feedforward Network. **(Left)** \mathbf{W} : 1st layer weight matrix. \mathbf{w} : second layer weight vector. \mathbf{c} : input biases. **(Right)** \mathbf{X} : input. \mathbf{b} : hidden layer bias.

Pre-Activation in One Unit

$\mathbf{W}^{(1)}$ is weight matrix for input-hidden connections.

$$\mathbf{W}^{(1)} = \begin{bmatrix} \mathbf{w}_{11} & \mathbf{w}_{12} \end{bmatrix}$$

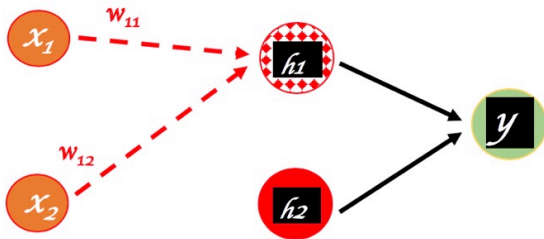


Figure: Connection weights from input to hidden in the 2×2 matrix \mathbf{W} are indexed with i (hidden unit index) and j (input unit index). We refer to the matrix as $\mathbf{W}^{(1)}$ to denote it is the first layer matrix (input-to-hidden). For simplification, bias is dropped.

Pre-Activation in One Unit: More Connection Weights

$\mathbf{W}^{(1)}$ is weight matrix for input-hidden connections.

$$\mathbf{W}^{(1)} = \begin{matrix} \mathbf{w}_{11} & \mathbf{w}_{12} \\ \mathbf{w}_{21} & \mathbf{w}_{22} \end{matrix}$$

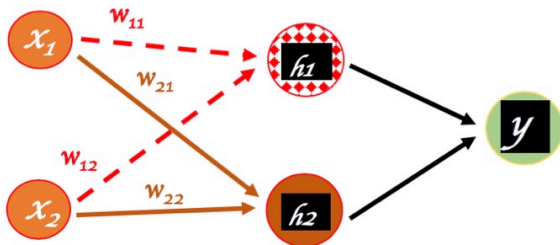


Figure: Connection weights from input to hidden in the 2×2 matrix \mathbf{W} are indexed with i (hidden unit index) and j (input unit index). We refer to the matrix as $\mathbf{W}^{(1)}$ to denote it is the first layer matrix (input-to-hidden).

Calculating a Feedforward Network (Compact)

1: 1-Hidden Layer Feedforward Network

$$\mathbf{h} = f^{(1)}(\mathbf{x}; \mathbf{W}, \mathbf{c})$$

$$\mathbf{y} = f^{(2)}(\mathbf{h}; \mathbf{w}, b)$$

The Whole **feedforward network** then is:

$$\mathbf{f} = (\mathbf{x}; \mathbf{W}, \mathbf{c}, \mathbf{w}, b)$$

Computing Hidden Layer

- Let's call $f^{(1)} : g$, and its input: z , so that we have: $g(z)$.
- g will be a nonlinear function, say a Rectified Linear Unit (ReLU), defined as: $g(z) = \max(0, z)$.
- The input $z = \mathbf{W}^T \mathbf{x} + \mathbf{c}$. \mathbf{W} : weight matrix.
- Two things happen: (1) The weighted summing, and (2) applying the activation function.

2: Computing Hidden Layer

$$\mathbf{h} = g(\mathbf{W}^T \mathbf{x} + \mathbf{c})$$

Rectified Linear Unit (ReLU)

- For g , we use a **non-linear activation function** like ReLU:

3: ReLU Non-Linear Activation Function

$$g(x) = \max(0, x)$$

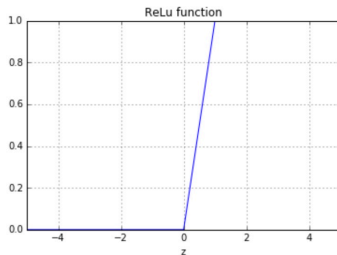


Figure: Rectified Linear Unit (ReLU). We use ReLU for hidden layer activations

Computing Output Layer

- Let's call $f^{(2)} : o$.
- Its input is \mathbf{h} , so that we have: $o(\mathbf{h})$.
- o will be a sigmoid (since we do binary activation here).
- For multiclass, we use softmax.

4: Computing Output Layer

Recall:

$$\mathbf{h} = g(\mathbf{W}^T \mathbf{x} + \mathbf{c})$$

Now for output:

$$o = \mathbf{w}^T \mathbf{h} + b.$$

Components of a Feedforward Network (For Solving XOR) I

$$\begin{aligned} \mathbf{W} &= \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} & \mathbf{X} &= \begin{matrix} & \mathbf{x}_1 & \mathbf{x}_2 \\ \begin{bmatrix} 0 & 0 \\ 0 & 1 \\ 1 & 0 \\ 1 & 1 \end{bmatrix} \end{matrix} \\ \mathbf{c} &= \begin{bmatrix} 0 \\ -1 \end{bmatrix} & \mathbf{b} &= \begin{bmatrix} 0 \end{bmatrix} \\ \mathbf{w} &= \begin{bmatrix} 1 \\ -2 \end{bmatrix} \end{aligned}$$

Figure: Ingredients of the Feedforward Network. **(Left)** \mathbf{W} : 1st layer weight matrix. \mathbf{w} : second layer weight vector. \mathbf{c} : input biases. **(Right)** \mathbf{X} : input. \mathbf{b} : hidden layer bias.

Calculating The Network II

We can now walk through the way that the model processes a batch of inputs. Let \mathbf{X} be the design matrix containing all four points in the binary input space, with one example per row:

$$\mathbf{X} = \begin{bmatrix} 0 & 0 \\ 0 & 1 \\ 1 & 0 \\ 1 & 1 \end{bmatrix}. \quad (6.7)$$

The first step in the neural network is to multiply the input matrix by the first layer's weight matrix:

$$\mathbf{XW} = \begin{bmatrix} 0 & 0 \\ 1 & 1 \\ 1 & 1 \\ 2 & 2 \end{bmatrix}. \quad (6.8)$$

Next, we add the bias vector \mathbf{c} , to obtain

$$\begin{bmatrix} 0 & -1 \\ 1 & 0 \\ 1 & 0 \\ 2 & 1 \end{bmatrix}. \quad (6.9)$$

Figure: Calculating the Feedforward I. (Goodfellow et al., 2016, p. 176)

Calculating The Network III

In this space, all of the examples lie along a line with slope 1. As we move along this line, the output needs to begin at 0, then rise to 1, then drop back down to 0. A linear model cannot implement such a function. To finish computing the value of \mathbf{h} for each example, we apply the rectified linear transformation:

$$\begin{bmatrix} 0 & 0 \\ 1 & 0 \\ 1 & 0 \\ 2 & 1 \end{bmatrix} \cdot \quad (6.10)$$

This transformation has changed the relationship between the examples. They no longer lie on a single line. As shown in figure 6.1, they now lie in a space where a linear model can solve the problem.

We finish by multiplying by the weight vector \mathbf{w} :

$$\begin{bmatrix} 0 \\ 1 \\ 1 \\ 0 \end{bmatrix} \cdot \quad (6.11)$$

Figure: Calculating the Feedforward II. (Goodfellow et al., 2016, p. 176)

Sigmoid Units for Bernoulli Output Distributions

- Used for tasks requiring predicting a **binary value** for y .
- Example: **positive** vs. **negative** sentiment.

5: Sigmoid Function

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

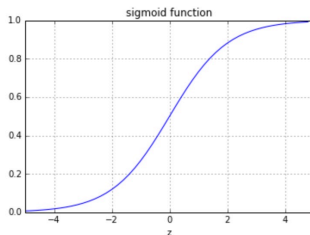


Figure: A plot of sigmoid.

6: Properties of Sigmoid

As activation becomes very small (with $e^{\text{very_large_number}}$), it goes to zero:

$$a \rightarrow -\infty : \sigma(a) \rightarrow 0$$

As activation becomes very large (with $e^{-\text{very_large_number}}$), it goes to 1:

$$a \rightarrow \infty : \sigma(a) \rightarrow 1$$

If $a = 0$, the function outputs $\frac{1}{2}$

The function is differentiable, with a nice form:

$$\Delta\sigma(a) = \sigma(a)(1 - \sigma(a))$$

Sigmoid Code Example I

```
1 import numpy as np
2 def sigmoid(x, derivative=False):
3     return x*(1-x) if derivative else 1/(1+np.exp(-x))
4
5 """
6 Note 1: We threshold value of activation a at -1 from below
7 (which will be what we will get if we used an activation
8 function like tanh [outputs values between -1 and 1] from previous layer. If output
9 activation came from a ReLu, it will be bounded by 0/zero from below)
10 """
11 a=0.01
12 print(sigmoid(a))
```

0.502499979167

```
1 a=1000
2 print(sigmoid(a))
```

1.0

```
1 a=-0.5
2 print(sigmoid(a))
```

0.377540668798

Sigmoid Code Example II

```
1 import numpy as np
2 def sigmoid(x, derivative=False):
3     return x*(1-x) if derivative else 1/(1+np.exp(-x))
4
5 """
6 Note 2: The function can take an array, although as an output unit it is
7 used over a single unit for binary classification
8 """
9 a=np.array([0.01, 0.2, 0.5, 0.8, 1.0, 2.5, 5.0, 100.0, 5000.0])
10 print(sigmoid(a))
```

```
[ 0.50249998  0.549834    0.62245933  0.68997448  0.73105858  0.92414182
  0.99330715  1.          1.          ]
```

Softmax Units for Categorical Output Distributions

- A **Categorical distribution** (also called generalized Bernoulli or Multinoulli) is a **probability distribution over a discrete variable with n possible outcomes**.
- Example: **{joy, sadness, anger, surprise}** for emotion is an example.
- We can use the **softmax** function for this.
- **Softmax is often used as the output of a classifier**, to represent a probability distribution of n different classes.
- To calculate a softmax, we produce a vector \hat{y} , with $\hat{y}_i = P(y = i|x)$:

Softmax Output

- each element of \hat{y}_i is between 0 and 1.
- The **entire vector \hat{y} sums to 1** so that it represents a valid probability distribution.

7: Softmax

First, a linear layer predicts unnormalized log probabilities:

$$z = W^T h + b$$

where

$$z_i = \log \hat{P}(y = i|x)$$

Then the softmax can **exponentiate and normalize** z to obtain \hat{y} :

$$\text{softmax}(z)_i = \frac{\exp(z_i)}{\sum_c \exp(z_c)}.$$

Where the **sum is over all the units/classes** (= same number of classes we are predicting).

We then predict the class with the **highest predicted probability**.