# Gradient Descent

## Towards Neural Networks

Justin Stevens
Undergraduate AI Society
April 2nd, 2019

# Outline

1. Decision Making
   - Perceptrons
   - Activation Functions

2. Classifying Digits through MNIST

# Should I Stay or Should I Go?

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| Ticket Prices | Availability | Interest | $\bar{\mathbf{x}}$ | $\bar{\mathbf{w}} \cdot \bar{\mathbf{x}}$ |
|---|---|---|---|---|
| Cheap | Yes | Yes | $(1, 1, 1)$ | 10 |
| Cheap | No | No | $(1, 0, 0)$ | 1 |
| Cheap | Yes | No | $(1, 1, 0)$ | 7 |
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We can now define my **activation threshold**, $t$, which will determine whether or not I go to the game, represented in binary.

# Formula for Decision Making

The general formula for my decision to go to the Oilers game is

$$\text{output} = \begin{cases} 0 & \text{if } \bar{\mathbf{w}} \cdot \bar{\mathbf{x}} < t \\ 1 & \text{if } \bar{\mathbf{w}} \cdot \bar{\mathbf{x}} \geq t. \end{cases}$$

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For instance, if $t = 9$, we see I'll only go if I'm both available and interested. If $t = 7$, I'll also go if the tickets are cheap and I'm available:

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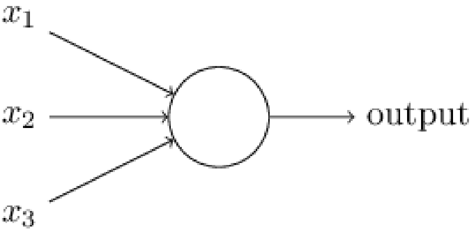


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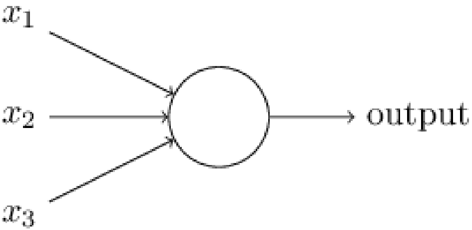


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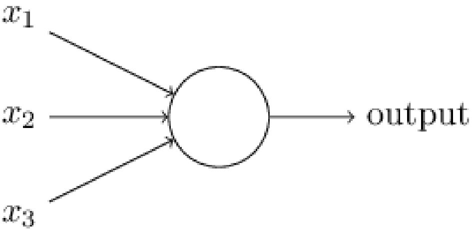


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Each of these lines collect evidence and are weighted to produce an output. In practice, our inputs and outputs don't necessarily have to be binary; they can be real-valued. We therefore have to define a new activation function.

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Instead of comparing our weighted sum to a threshold, we instead *add* a bias, $b$, to our weighted sum. We write this as $\bar{\mathbf{w}} \cdot \bar{\mathbf{x}} + b$ instead.

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Graphically, we can see:

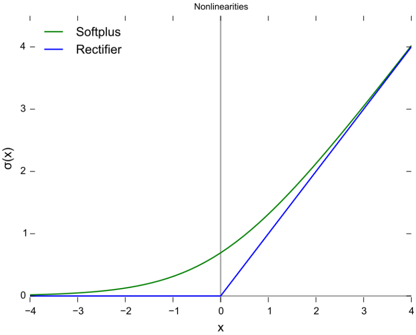


Figure 2: Rectifier, and a smooth approximation $\log(1 + e^x)$. (*Source: Wikipedia*).

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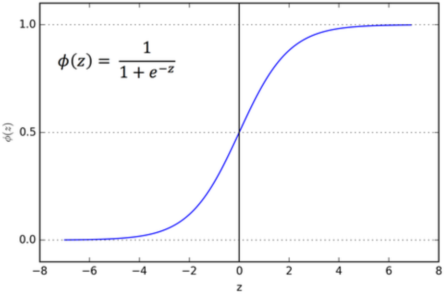


Figure 3: As $z \to \infty$, we see $\sigma(z) \to 1$. Alternatively, as $z \to -\infty$, $\sigma(z) \to 0$. (*Source: Towards Data Science*).

# Outline

# Example Images

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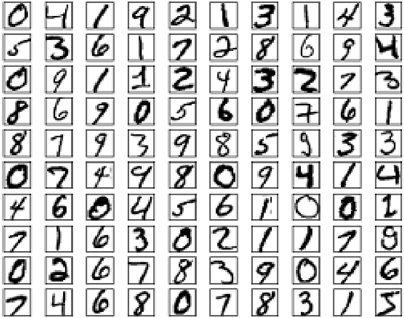

Figure 4: How would you devise a system for a **computer** to classify the digits? How can we best utilize the data set, known as MNIST? (*Source: Nielsen*)

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We'll build a model from the training images that will learn to classify digits!

# What we're building towards

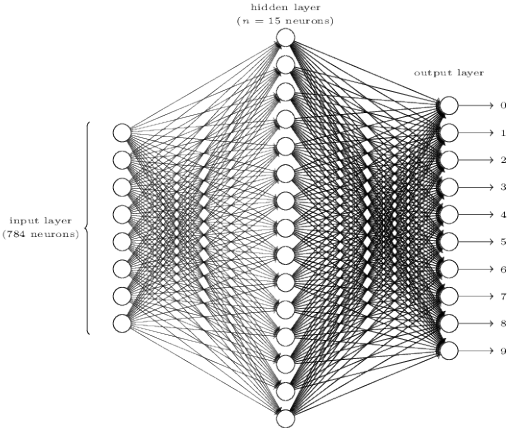


Figure 5: A simple neural network structure. The input vectors on the left hand side have $28 \times 28 = 784$ inputs for each pixel, and the output layer has 10 digits. (*Source: Nielsen*)

# Extending our Model

All of our weights and bias will be initialized from a normal distribution with mean 0 and standard deviation 1.

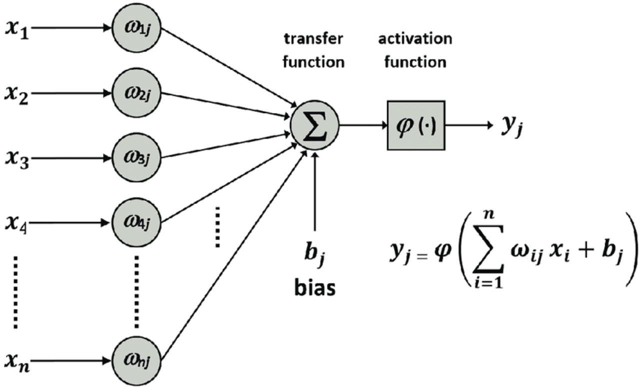


Figure 6: *Source: Daniel Alvarez, InTech*

# Hidden Layer

The role of the **hidden layer** is to hold intermediate calculations. These will in turn be used to compute the output layer. To produce the hidden layer, we must have an $784 \times 15$ weight matrix, as seen below:

$$W = \begin{pmatrix} w_{11} & w_{12} & \cdots & w_{1,784} \\ w_{21} & w_{22} & \cdots & w_{2,784} \\ \vdots & \vdots & \ddots & \vdots \\ w_{15,1} & w_{15,2} & \cdots & w_{15,784} \end{pmatrix}, \quad \mathbf{x} = \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ \vdots \\ x_{784} \end{pmatrix}, \quad \mathbf{b} = \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_{15} \end{pmatrix}.$$

We take the dot product of each **row** with our input vector $\mathbf{x}$. We then add our bias vector, $\mathbf{b}$, which is $15 \times 1$. We finally apply our activation:

$$\mathbf{h} = \sigma(W\mathbf{x} + \mathbf{b}).$$

Notice the sigmoid function is applied component wise.

# Output Layer

We must now define a transformation from $\mathbb{R}^{15}$ to $\mathbb{R}^{10}$, which we can do using a $10 \times 15$ weight matrix $\hat{W}$. We can then add a $10 \times 1$ bias vector, $\hat{\mathbf{b}}$.

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Notice the sum of these values will always be 1. The full computation is

$$\mathbf{f} = \hat{W}\mathbf{h} + \mathbf{b}, \quad \mathbf{o} = \text{softmax}\left(\mathbf{f}\right).$$

# One Hot Encoding

Once we've computed the output, we need a way to compare it to our desired result. However, $\mathbf{o}$ is a $10 \times 1$ vector, whereas our desired digit $y_{\text{train}}(\mathbf{x})$ is a scalar. We therefore encode the digit as a $10 \times 1$ vector:

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$$\begin{array}{ccccc} \begin{pmatrix}1\\0\\0\\\vdots\\0\end{pmatrix} & \begin{pmatrix}0\\1\\0\\\vdots\\0\end{pmatrix} & \begin{pmatrix}0\\0\\1\\\vdots\\0\end{pmatrix} & \cdots & \begin{pmatrix}0\\0\\0\\\vdots\\1\end{pmatrix} \\ \hline 0 & 1 & 2 & \cdots & 9 \end{array}$$

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The code for this is relatively simple:

```
y_test=keras.utils.to_categorical(y_test, num_classes=10)
y_train=keras.utils.to_categorical(y_train, num_classes=10)
```

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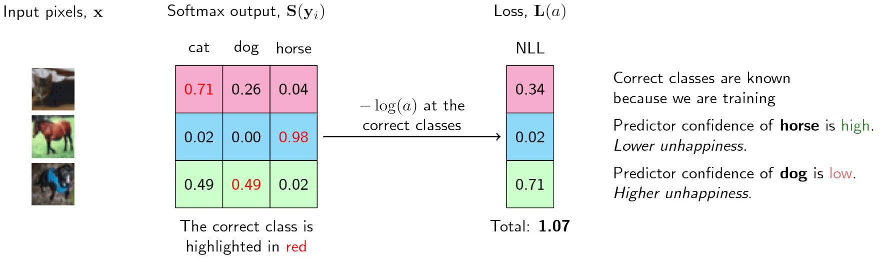


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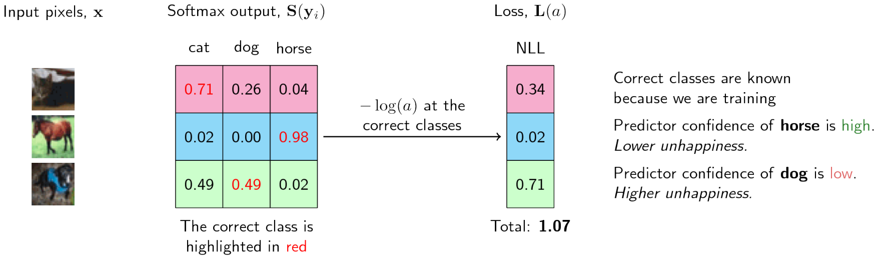


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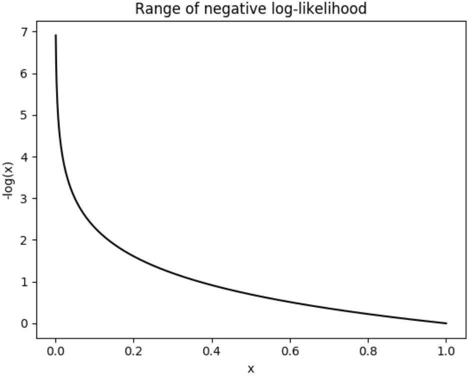
To compute the loss for an individual training example, $\mathbf{x}$, with one-hot encoded label $y_{\text{train}}(\mathbf{x})$, and output $\mathbf{o}$, we compute

$$L(\mathbf{x}) = -y_{\text{train}}(\mathbf{x}) \cdot \log \mathbf{o} = -\log(o_j),$$

where $j$ is the true label.

# Graph of Negative Log

Recall $L(\mathbf{x}) = -\log(o_j)$. Since $o_j$ is between 0 and 1, we can graph the function, noting it approaches 0 as $o_j \to 1$, and goes to $\infty$ as $o_j \to 0$.

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# Summarizing the Loss Function

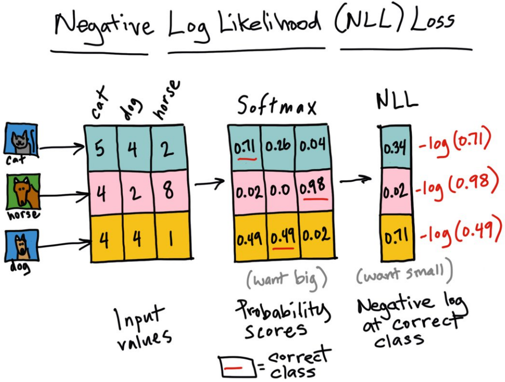


Figure 9: *Source: Micheleen Harris*

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$$L = -\log\left(o_j\right), \quad o_j = \frac{e^{f_j}}{e^{f_1} + e^{f_2} + \cdots + e^{f_{10}}}.$$

Then $\frac{\partial L}{\partial f_j} = \frac{\partial L}{\partial o_j}\frac{\partial o_j}{\partial f_j} = -\frac{1}{o_j}\frac{\partial o_j}{\partial f_j}$. Using the quotient rule and some algebra,

# Backpropagation

In our hidden layer, we have $784 \times 15 + 15 \times 1 = 11,775$ weights and biases to train on. In the output layer, we only have $15 \times 10 + 10 \times 1 = 160$. We'll answer the question: how much does our loss function depend on these parameters? To answer this, we need the chain rule from calculus:

$$L = -\log\left(o_j\right), \quad o_j = \frac{e^{f_j}}{e^{f_1} + e^{f_2} + \cdots + e^{f_{10}}}.$$

Then $\frac{\partial L}{\partial f_j} = \frac{\partial L}{\partial o_j}\frac{\partial o_j}{\partial f_j} = -\frac{1}{o_j}\frac{\partial o_j}{\partial f_j}$. Using the quotient rule and some algebra,

$$\begin{aligned}
\frac{\partial L}{\partial f_j} &= -\frac{1}{o_j}\frac{\left(e^{f_1} + \cdots + e^{f_{10}}\right)e^{f_j} - e^{f_j}e^{f_j}}{\left(e^{f_1} + \cdots + e^{f_{10}}\right)^2} \\
&= -\frac{e^{f_1} + \cdots + e^{f_{10}}}{e^{f_j}} \cdot \frac{e^{f_j}\left(e^{f_1} + e^{f_2} + \cdots + e^{f_{10}} - e^{f_j}\right)}{\left(e^{f_1} + \cdots + e^{f_{10}}\right)^2} \\
&= -\frac{e^{f_1} + \cdots + e^{f_{10}} - e^{f_j}}{e^{f_1} + \cdots + e^{f_{10}}} = -\left(1 - o_j\right) = o_j - 1.
\end{aligned}$$

# References

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