Gradient Descent

Towards Neural Networks

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Undergraduate AI Society
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Outline

1. Decision Making
   - Perceptrons
   - Activation Functions
2. Classifying Digits through MNIST
3. Improvements

Should I Stay or Should I Go?

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Cheap	Yes	Yes	$(1, 1, 1)$	10
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Cheap	Yes	No	$(1, 1, 0)$	7
Cheap	No	Yes	$(1, 0, 1)$	4
Expensive	Yes	Yes	$(0, 1, 1)$	9
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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:

Ticket Prices	Availability	Interest	$\bar{\mathbf{x}}$	$\bar{\mathbf{x}} \cdot \bar{\mathbf{w}}$
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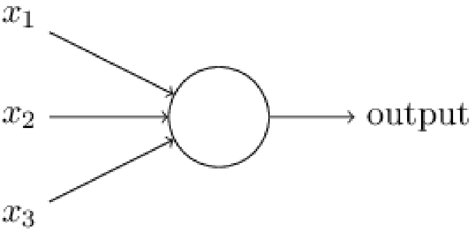

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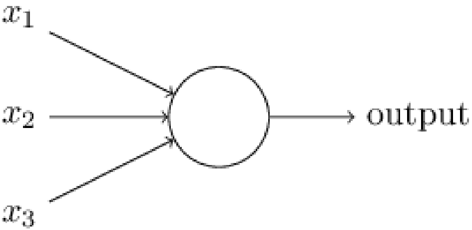

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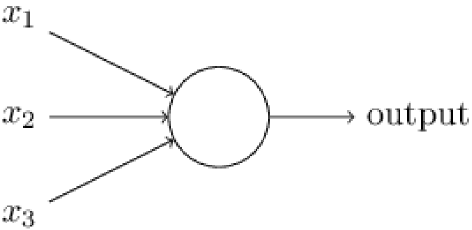

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Each of these lines collect evidence and are weighted to produce an output. In practice, our inputs and outputs don't necessarily have to be binary; they can be real-valued. We therefore have to define a new activation function.

Introducing the Bias

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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This is known as the *heaviside step function*. We'll extend our model to multiple outputs soon, but first we'll examine other activation functions.

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Graphically, we can see:

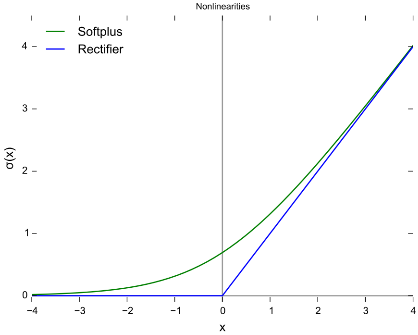

Figure 2: Rectifier, and a smooth approximation $\log(1 + e^x)$. (*Source: Wikipedia*).

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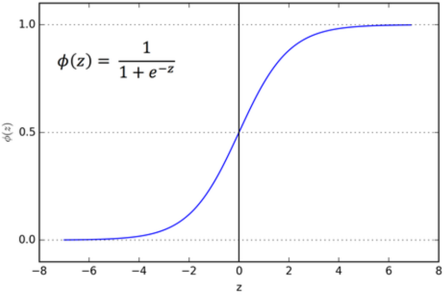

Figure 3: As $z \to \infty$, we see $\sigma(z) \to 1$. Alternatively, as $z \to -\infty$, $\sigma(z) \to 0$. (*Source: Towards Data Science*).

Outline

Example Images

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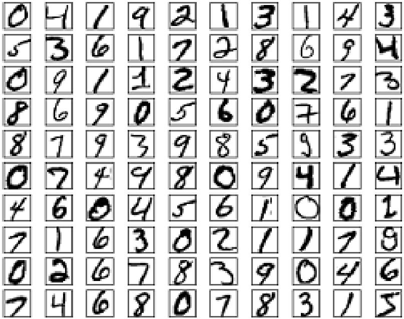

Figure 4: How would you devise a system for a **computer** to classify the digits? How can we best utilize the data set, known as MNIST? (*Source: Nielsen*)

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

What we're building towards

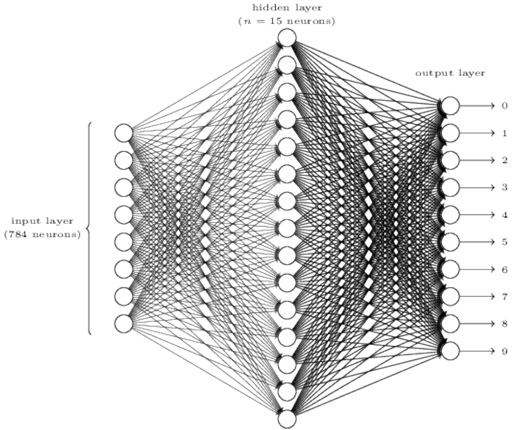

Figure 5: A simple neural network structure. The input vectors on the left hand side have $28 \times 28 = 784$ inputs for each pixel, and the output layer has 10 digits. (*Source: Nielsen*)

Extending our Model

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

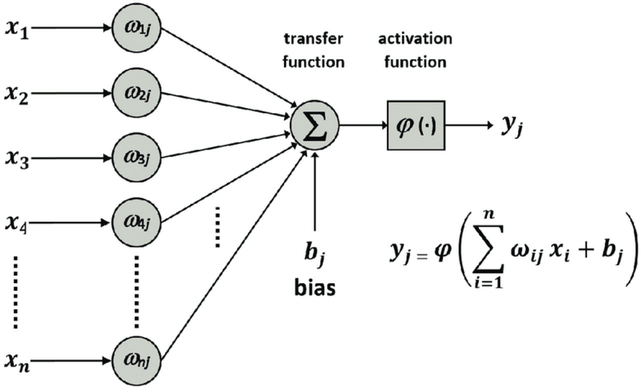

Figure 6: *Source: Daniel Alvarez, InTech*

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 784×15 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 15×1. We finally apply our activation:

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

Notice the sigmoid function is applied component wise.

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$$\text{softmax}(\mathbf{z})_j = \frac{e^{z_j}}{\sum_{k=1}^{10} e^{z_k}}, \quad 1 \leq j \leq 10.$$

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

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 10×1 vector, whereas our desired digit $y_{\text{train}}(\mathbf{x})$ is a scalar. We therefore encode the digit as a 10×1 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} \\
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0 & 1 & 2 & \cdots & 9
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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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Input pixels, $\mathbf{x}$

Softmax output, $\mathbf{S}(\mathbf{y}_i)$

cat	dog	horse
0.71	0.26	0.04
0.02	0.00	0.98
0.49	0.49	0.02

The correct class is highlighted in red

$-\log(a)$ at the correct classes $\longrightarrow$

Loss, $\mathbf{L}(a)$

NLL
0.34
0.02
0.71

Total: **1.07**

Correct classes are known because we are training

Predictor confidence of **horse** is high. *Lower unhappiness.*

Predictor confidence of **dog** is low. *Higher unhappiness.*

Figure 7: *Source: LJ Mirand*

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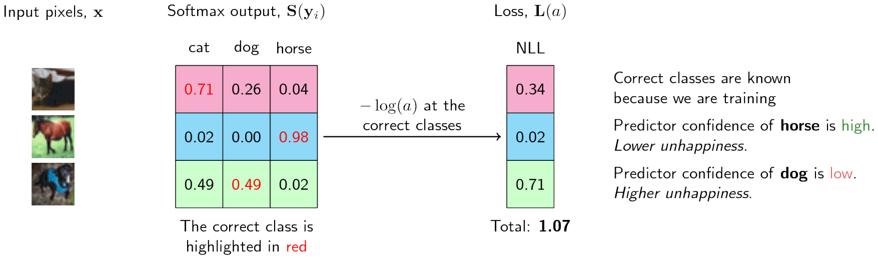

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To compute the loss for an individual training example, $\mathbf{x}$, with one-hot encoded label $y_{\text{train}}(\mathbf{x})$, and output $\mathbf{o}$, we compute

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

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 ∞ as $o_j \to 0$.

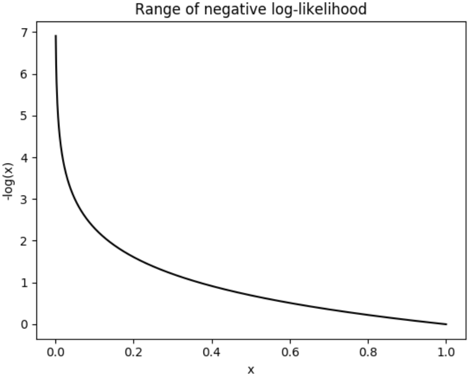

Figure 8: *Source: LJ Mirand*

Summarizing the Loss Function

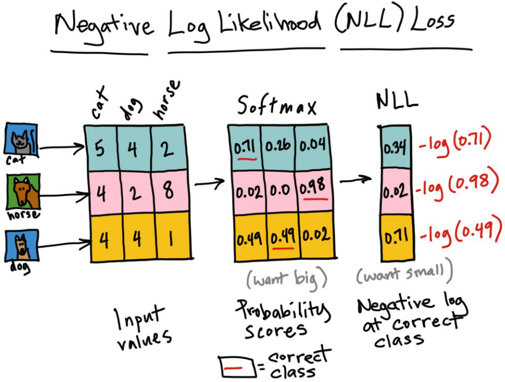

Figure 9: *Source: Micheleen Harris*

Gradient Descent Intuition

Our goal is to minimize loss with respect to weights and biases. To simplify the model, let's assume C is a function of two variables: v_1 and v_2.

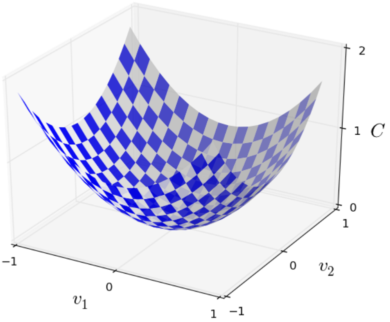

Figure 10: *Source: Nielsen*

Gradient Descent II

We see how much C changes as we nudge v_1 and v_2. Approximating,

$$\Delta C \approx \frac{\partial C}{\partial v_1}\Delta v_1 + \frac{\partial C}{\partial v_2}\Delta v_2.$$

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We find the optimal way to adjust Δv_1 and Δv_2 so that ΔC is negative. We define $\Delta v = \binom{\Delta v_1}{\Delta v_2}$ and the **gradient** vector $\nabla C = \begin{pmatrix} \frac{\partial C}{\partial v_1} & \frac{\partial C}{\partial v_2} \end{pmatrix}^T$.

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$$\Delta C \approx \nabla C \cdot \Delta v.$$

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$$\Delta C \approx \frac{\partial C}{\partial v_1}\Delta v_1 + \frac{\partial C}{\partial v_2}\Delta v_2.$$

We find the optimal way to adjust Δv_1 and Δv_2 so that ΔC is negative. We define $\Delta v = \binom{\Delta v_1}{\Delta v_2}$ and the **gradient** vector $\nabla C = \begin{pmatrix} \frac{\partial C}{\partial v_1} & \frac{\partial C}{\partial v_2} \end{pmatrix}^T$.Therefore,

$$\Delta C \approx \nabla C \cdot \Delta v.$$

By the Cauchy-Schwartz inequality, the direction of greatest descent is $\Delta v = -\lambda \nabla C$. In this case, $\Delta C \approx \nabla C \cdot -\lambda \nabla C = -\lambda \left\|\nabla C\right\|^2 \ll 0$.

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We therefore update $v \to v' = v - \lambda \nabla C$, where λ is the **learning rate**. We iterate this process in the hopes of finding a local minimum of C. This process can fairly easily generalize from 2 variables to n variables if we wish.

Gradient Descent III

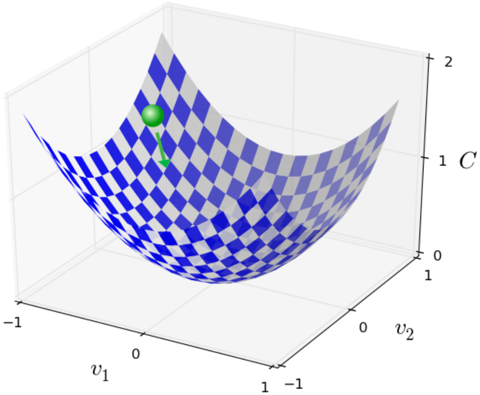

Figure 11: *Source: Nielsen*

Gradient Descent IV

Our general rule for updating weights and biases in our neural network is

$$w_k \to w_k' = w_k - \eta \frac{\partial L}{\partial w_k}, \quad b_\ell \to b_\ell' = b_\ell - \eta \frac{\partial L}{\partial b_\ell}.$$

In practice, updating our weights at every step is subject to stochastic error.

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We can rewrite our update steps as $\begin{cases} w_k \to & w_k' = w_k - \frac{\eta}{m} \sum_{i=1}^{m} \frac{\partial L_{X_i}}{\partial w_k} \\ b_\ell \to & b_\ell' = b_\ell - \frac{\eta}{m} \sum_{i=1}^{m} \frac{\partial L_{X_i}}{\partial w_k} \end{cases}.$

Backpropagation Part I

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 $15 \times 10 + 10 \times 1 = 160$.

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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,

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

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

We've now computed how much our loss function depends upon the final activations before applying the softmax. We now go back a layer and see how much L depends upon $\hat{W}$ and $\hat{b}$, and store these results in a gradient.

Backpropagation Part III

We can write this as $\mathbf{f} = \begin{pmatrix} \hat{w}_{11} & \hat{w}_{12} & \cdots & \hat{w}_{1,15} \\ \hat{w}_{21} & \hat{w}_{22} & \cdots & \hat{w}_{2,15} \\ \vdots & \vdots & \vdots & \vdots \\ \hat{w}_{10,1} & \hat{w}_{10,2} & \cdots & \hat{w}_{10,15} \end{pmatrix} \begin{pmatrix} h_1 \\ h_2 \\ \vdots \\ \vdots \\ h_{15} \end{pmatrix} + \begin{pmatrix} \hat{b}_1 \\ \hat{b}_2 \\ \vdots \\ \hat{b}_{10} \end{pmatrix}.$

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We can similarly see $\dfrac{\partial L}{\partial b_k} = \displaystyle\sum_{i=1}^{10} \dfrac{\partial L}{\partial f_i} \dfrac{\partial f_i}{\partial b_k} = \dfrac{\partial L}{\partial f_k} \dfrac{\partial f_k}{\partial b_k} = \begin{cases} o_k & \text{if } k \neq j \\ o_k - 1 & \text{if } k = j. \end{cases}$.

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Finally, we can observe $\frac{\partial f_i}{\partial h_k} = \hat{w}_{ik}$ by the way we set up the matrix. We store all of these values in a gradient table for easy access later. This is a core feature of **dynamic programming**, which is essential in this program.

Backpropagation IV

Recall in the hidden layer, $h = \sigma(W\bar{x} + \bar{b})$, where

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

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By matrix multiplication, $h_k = \sigma(w_{k1}x_1 + w_{k2}x_2 + \cdots + w_{k,784}x_{784} + b_k)$. By the chain rule, we note $w_{k\ell}$ is fed into every final layer, therefore

$$\begin{aligned} \frac{\partial L}{\partial w_{k\ell}} &= \sum_{i=1}^{10} \frac{\partial L}{\partial f_i} \frac{\partial f_i}{\partial h_k} \frac{\partial h_k}{\partial w_{k\ell}} \\ &= \left(\sum_{i \neq j} o_i w_{ik} + (o_j - 1) w_{jk} \right) \frac{\partial h_k}{\partial w_{k\ell}}. \end{aligned}$$

Backpropagation Finale

Let $g_k = w_{k1}x_1 + w_{k2}x_2 + \cdots + w_{k,784}x_{784} + b_k$. Then $h_k = \sigma(g_k)$ hence

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Recall $\sigma(z) = \frac{1}{1+e^{-z}}$, so $\frac{d}{dz}\sigma(z) = \frac{e^{-z}}{1+e^{-z}} \cdot \frac{1}{1+e^{-z}} = (1 - \sigma(z))\,\sigma(z)$.

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Similarly, we see $\frac{\partial h_k}{\partial b_k} = (1 - \sigma(g_k))\,\sigma(g_k)$, since $\frac{\partial g_k}{\partial b_k} = 1$.

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$$\frac{\partial L}{\partial w_{k\ell}} = \left(\sum_{i\neq j} o_i w_{ik} + (o_j - 1)w_{jk}\right)(1-\sigma(g_k))\,\sigma(g_k)\mathbf{x}_\ell$$

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Outline

1. Decision Making
2. Classifying Digits through MNIST
3. Improvements
   - Overfitting
   - References

Overfitting

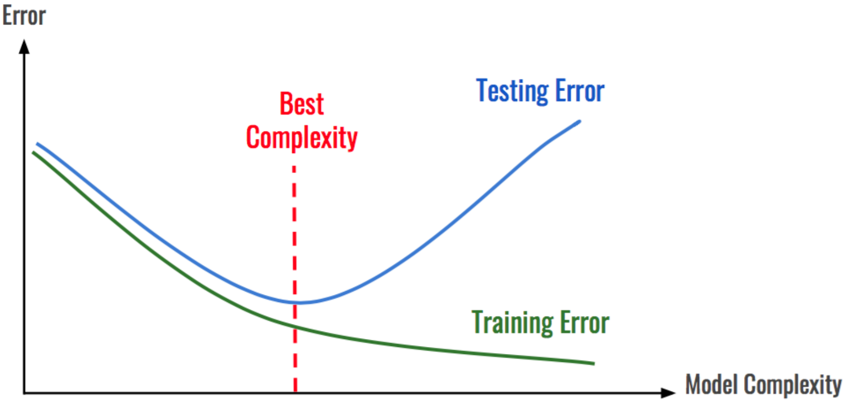

Figure 12: *Source: Hacker Noon*

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