Gradient Descent

Towards Neural Networks

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Undergraduate AI Society
April 2nd, 2019

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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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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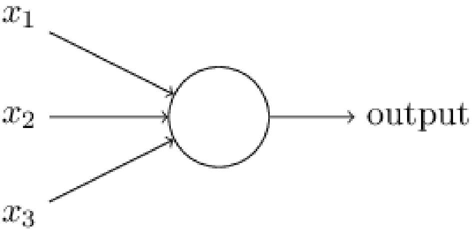

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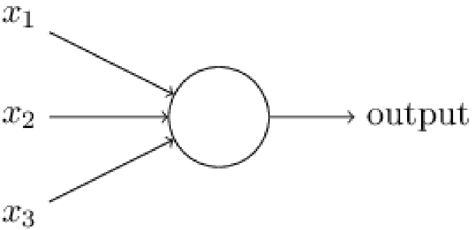

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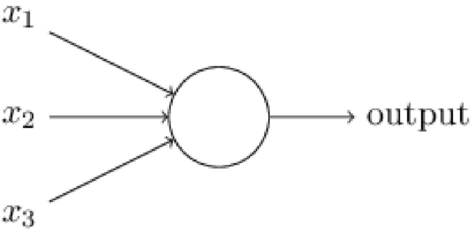

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Each of these lines collect evidence and are weighted to produce an output. In practice, our inputs and outputs don't necessarily have to be binary; they can be real-valued. We therefore have to define a new activation function.

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:

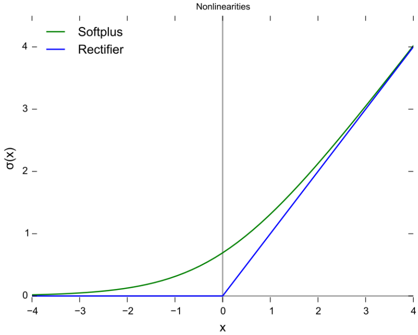

Figure 2: Rectifier, and a smooth approximation $\log(1 + e^x)$. (*Source: Wikipedia*).

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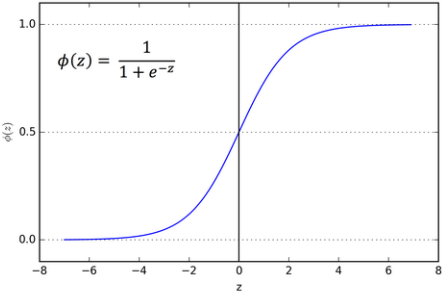

Figure 3: As $z \to \infty$, we see $\sigma(z) \to 1$. Alternatively, as $z \to -\infty$, $\sigma(z) \to 0$. (*Source: Towards Data Science*).

Outline

Example Images

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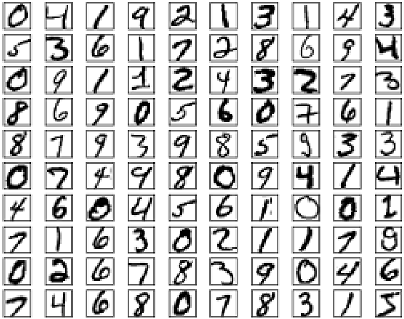

Figure 4: How would you devise a system for a **computer** to classify the digits? How can we best utilize the data set, known as MNIST? (*Source: Nielsen*)

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

What we're building towards

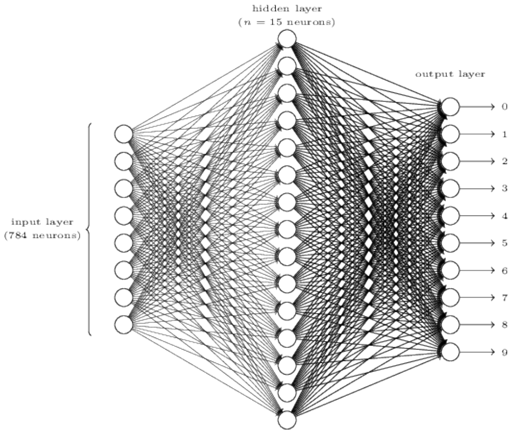

Figure 5: A simple neural network structure. The input vectors on the left hand side have $28 \times 28 = 784$ inputs for each pixel, and the output layer has 10 digits. (*Source: Nielsen*)

Extending our Model

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

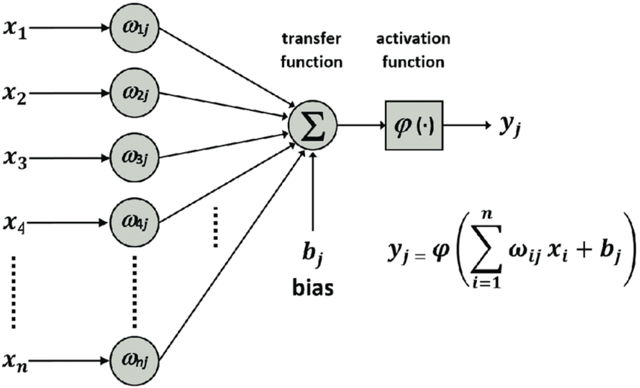

Figure 6: *Source: Daniel Alvarez, InTech*

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

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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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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)
```

Negative Log Likelihood

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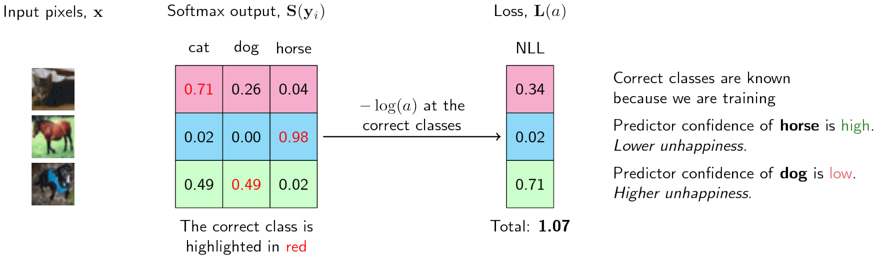

Figure 7: *Source: LJ Mirand*

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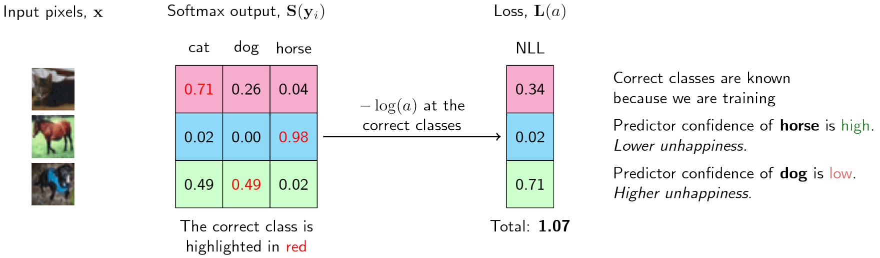

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To compute the loss for an individual training example, $\mathbf{x}$, with one-hot encoded label $y_{\text{train}}(\mathbf{x})$, and output $\mathbf{o}$, we compute

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

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 $o_j \to 0$.

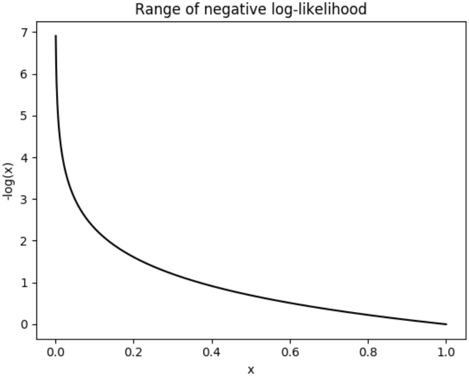

Figure 8: *Source: LJ Mirand*

Summarizing the Loss Function

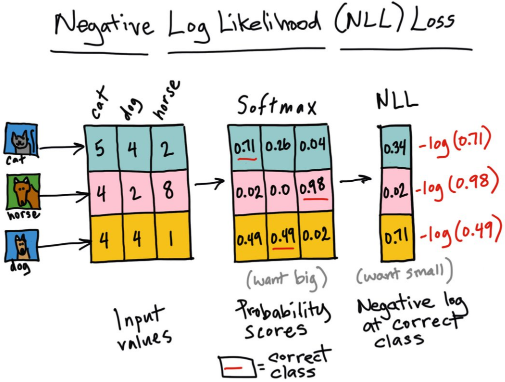

Figure 9: *Source: Micheleen Harris*

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.

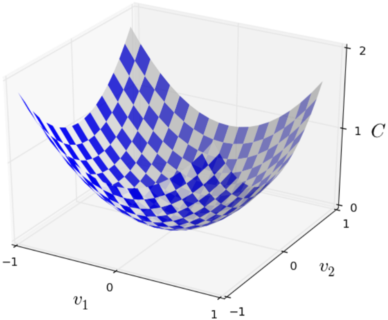

Figure 10: *Source: Nielsen*

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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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 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

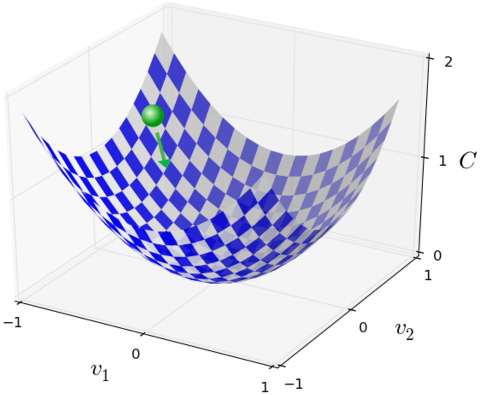

Figure 11: *Source: Nielsen*

Gradient Descent IV

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

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

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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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$$\begin{aligned}
\frac{\partial L}{\partial f_j} &= -\frac{1}{o_j}\frac{\left(e^{f_1} + \cdots + e^{f_{10}}\right)e^{f_j} - e^{f_j}e^{f_j}}{\left(e^{f_1} + \cdots + e^{f_{10}}\right)^2} \\
&= -\frac{e^{f_1} + \cdots + e^{f_{10}}}{e^{f_j}} \cdot \frac{e^{f_j}\left(e^{f_1} + e^{f_2} + \cdots + e^{f_{10}} - e^{f_j}\right)}{\left(e^{f_1} + \cdots + e^{f_{10}}\right)^2} \\
&= -\frac{e^{f_1} + \cdots + e^{f_{10}} - e^{f_j}}{e^{f_1} + \cdots + e^{f_{10}}} = -\left(1 - o_j\right) = o_j - 1.
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$$\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} \\
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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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Therefore, $\dfrac{\partial L}{\partial \hat{w}_{k\ell}} = \displaystyle\sum_{i=i}^{10} \frac{\partial L}{\partial f_i} \frac{\partial f_i}{\partial \hat{w}_{k\ell}} = \frac{\partial L}{\partial f_k} \frac{\partial f_k}{\partial \hat{w}_{k\ell}} = \begin{cases} o_k h_\ell & \text{if } k \neq j \\ (o_k - 1)\, h_\ell & \text{if } k = j \end{cases}$.

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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

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

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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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This process is one epoch. It's often helpful to pass our data through our training model multiple times to get the best weights and biases. For our optimizer, we'll use “tf.train.GradientDescentOptimizer(0.2)".

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If we wish to use a **varied** learning rate, we can use a different optimizer, such as *stochastic gradient descent*. We can then use "sgd", or an even more optimized version such as "adam".

Outline

Overfitting

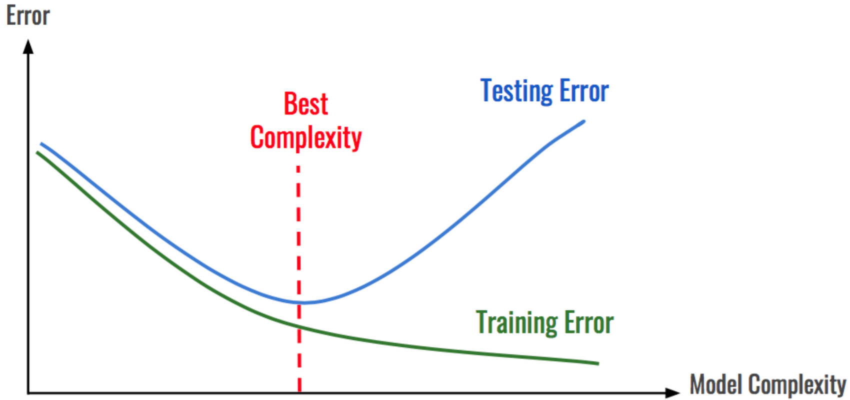

Figure 12: *Source: Hacker Noon*

References

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- LJ Mirand: Understanding softmax and the negative log-likelihood
- Towards Data Science: A Beginner's Guide to Neural Networks
- Deep Learning, Goodfellow et. al.
- 3d Visualizing a Neural Network
- Visualizing Gradient Descent
- Tensorflow Tutorials