Backpropagation Algorithm

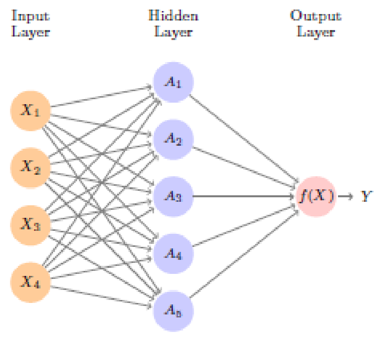
Subham Roy
Department of Computer Science and Engineering
University at Buffalo, Buffalo, NY 14260

1 Overview

A neural network is a series of algorithms that endeavors to recognize underlying relationships in a set of data through a process that mimics the way the human brain operates. In this sense, neural networks refer to systems of neurons, either organic or artificial in nature. Neural networks can adapt to changing input; so, the network generates the best possible result without needing to redesign the output criteria.

2 About Backpropagation Algorithm

Fitting neural networks are complex, and we have an overview here. The idea is to generalize much more complex networks. We start with the simple network depicted below –



In the model, the hidden layer computes activations $A_k = h_k(X)$ that are nonlinear transformations of linear combinations of the inputs $X_1, X_2, \ldots, X_p$, and the parameters are $\beta = (\beta_0, \beta_1, \ldots, \beta_K)$, as well as each of the $w_k = (w_{k0}, w_{k1}, \ldots, w_{kp})$, $k = 1, \ldots, K$. Given observations (x_i, y_i), $i = 1, \ldots, n$, we could fit the model by solving a nonlinear least squares problem -

$$\underset{\{w_k\}_1^K,\ \beta}{\text{minimize}} \frac{1}{2}\sum_{i=1}^{n}(y_i - f(x_i))^2,$$

where

$$f(x_i) = \beta_0 + \sum_{k=1}^{K}\beta_k g\Big(w_{k0} + \sum_{j=1}^{p} w_{kj}x_{ij}\Big)$$

The objective in the first formula looks simple enough, but because of the nested arrangement of the parameters and the symmetry of the hidden units, it is not straightforward to minimize. Suppose we represent all the parameters in one long vector θ. Then we can rewrite the objective in the first formula as –

$$R(\theta) = \frac{1}{2}\sum_{i=1}^{n}(y_i - f_\theta(x_i))^2$$

where we make explicit the dependence on the parameters.
Now our objective is to move θ to decrease the objective $R(\theta)$. The gradient of $R(\theta)$, evaluated at some latest/current value gradient $\theta = \theta^m$, is the vector of partial derivatives at that point:

$$\nabla R(\theta^m) = \frac{\partial R(\theta)}{\partial \theta}\Big|_{\theta=\theta^m}$$

The superscript of $\theta = \theta^m$ means that after computing the vector of derivatives, we evaluate it at the latest/current θ^m. This gives the direction in θ-space in which $R(\theta)$ increases most rapidly. The idea of gradient descent is to move θ in the opposite direction since we wish to go backward:

$$\theta^m + 1 \leftarrow \theta^m - \rho\nabla R(\theta^m)$$

For a small value of the learning rate ρ, this step will decrease the objective $R(\theta)$; i.e., $R(\theta^{m+1}) \leqslant R(\theta^m)$. If the gradient vector is zero, then we may have arrived at a minimum of the objective. Since, $R(\theta) = \sum_{i=1}^{n} R_i(\theta) = \frac{1}{2}\sum_{i=1}^{n}(y_i - f_\theta(x_i))^2$ is a sum, its gradient is also a sum over the n observations, so now we will just examine one of the terms –

$$R_i(\theta) = \frac{1}{2}\Big(y_i - \beta_0 - \sum_{k=1}^{K}\beta_k g\big(w_{k0} + \sum_{j=1}^{p} w_{kj}x_{ij}\big)\Big)^2$$

To simplify the expressions to follow, we write – $z_{ik} = w_{k0} + \sum_{j=1}^{p} w_{kj}x_{ij}$

Firstly, we take the derivative with respect to β_k:

$$\begin{aligned}\frac{\partial R_i(\theta)}{\partial \beta_k} &= \frac{\partial R_i(\theta)}{\partial f_\theta(x_i)} \cdot \frac{\partial f_\theta(x_i)}{\partial \beta_k} \\ &= -(y_i - f_\theta(x_i)) \cdot g(z_{ik})\end{aligned}$$

And now we take the derivative with respect to w_{kj}:

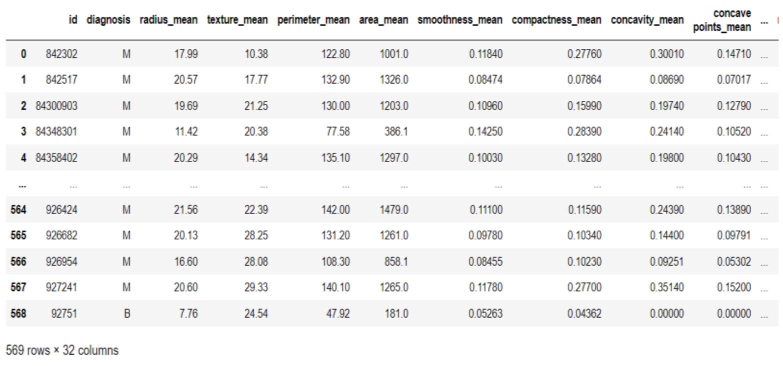
$$\begin{aligned}\frac{\partial R_i(\theta)}{\partial w_{kj}} &= \frac{\partial R_i(\theta)}{\partial f_\theta(x_i)} \cdot \frac{\partial f_\theta(x_i)}{\partial g(z_{ik})} \cdot \frac{\partial g(z_{ik})}{\partial z_{ik}} \cdot \frac{\partial z_{ik}}{\partial w_{kj}} \\ &= -(y_i - f_\theta(x_i)) \cdot \beta_k \cdot g'(z_{ik}) \cdot x_{ij}.\end{aligned}$$

Note that both these expressions contain the residual $(y_i - f_\theta(x_i))$. In the result for the derivative with respect to β_k, we see that a fraction of that residual gets attributed to each of the hidden units according to the value of $g(z_{ik})$. Then in the later derivative, we see a similar attribution to input j via hidden unit k. So, the act of differentiation assigns a fraction of the residual to each of the parameters via the chain rule of differentiation, a process commonly known as Backpropagation in Neural Networks.

3 Experiment

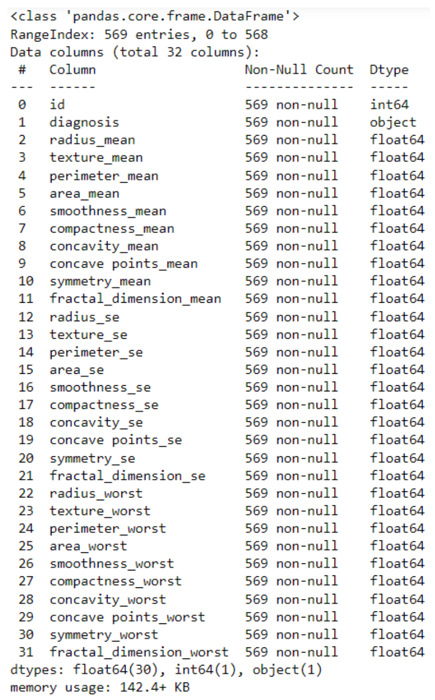
In this experiment, I used the Women Breast Cancer dataset from the url in Reference. Initially, we start with loading the Dataset and checking the dimensions and the number of variables within the Dataset. In this case, the dataset has 32 features and 569 rows.

Dataset description –



	id	diagnosis	radius_mean	texture_mean	perimeter_mean	area_mean	smoothness_mean	compactness_mean	concavity_mean	concave points_mean	...
0	842302	M	17.99	10.38	122.80	1001.0	0.11840	0.27760	0.30010	0.14710	...
1	842517	M	20.57	17.77	132.90	1326.0	0.08474	0.07864	0.08690	0.07017	...
2	84300903	M	19.69	21.25	130.00	1203.0	0.10960	0.15990	0.19740	0.12790	...
3	84348301	M	11.42	20.38	77.58	386.1	0.14250	0.28390	0.24140	0.10520	...
4	84358402	M	20.29	14.34	135.10	1297.0	0.10030	0.13280	0.19800	0.10430	...
...	...	...	...	...	...	...	...	...	...	...	...
564	926424	M	21.56	22.39	142.00	1479.0	0.11100	0.11590	0.24390	0.13890	...
565	926682	M	20.13	28.25	131.20	1261.0	0.09780	0.10340	0.14400	0.09791	...
566	926954	M	16.60	28.08	108.30	858.1	0.08455	0.10230	0.09251	0.05302	...
567	927241	M	20.60	29.33	140.10	1265.0	0.11780	0.27700	0.35140	0.15200	...
568	92751	B	7.76	24.54	47.92	181.0	0.05263	0.04362	0.00000	0.00000	...

569 rows × 32 columns



```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 569 entries, 0 to 568
Data columns (total 32 columns):
 #   Column                   Non-Null Count  Dtype  
---  ------                   --------------  -----  
 0   id                       569 non-null    int64  
 1   diagnosis                569 non-null    object 
 2   radius_mean              569 non-null    float64
 3   texture_mean             569 non-null    float64
 4   perimeter_mean           569 non-null    float64
 5   area_mean                569 non-null    float64
 6   smoothness_mean          569 non-null    float64
 7   compactness_mean         569 non-null    float64
 8   concavity_mean           569 non-null    float64
 9   concave points_mean      569 non-null    float64
 10  symmetry_mean            569 non-null    float64
 11  fractal_dimension_mean   569 non-null    float64
 12  radius_se                569 non-null    float64
 13  texture_se               569 non-null    float64
 14  perimeter_se             569 non-null    float64
 15  area_se                  569 non-null    float64
 16  smoothness_se            569 non-null    float64
 17  compactness_se           569 non-null    float64
 18  concavity_se             569 non-null    float64
 19  concave points_se        569 non-null    float64
 20  symmetry_se              569 non-null    float64
 21  fractal_dimension_se     569 non-null    float64
 22  radius_worst             569 non-null    float64
 23  texture_worst            569 non-null    float64
 24  perimeter_worst          569 non-null    float64
 25  area_worst               569 non-null    float64
 26  smoothness_worst         569 non-null    float64
 27  compactness_worst        569 non-null    float64
 28  concavity_worst          569 non-null    float64
 29  concave points_worst     569 non-null    float64
 30  symmetry_worst           569 non-null    float64
 31  fractal_dimension_worst  569 non-null    float64
dtypes: float64(30), int64(1), object(1)
memory usage: 142.4+ KB
```

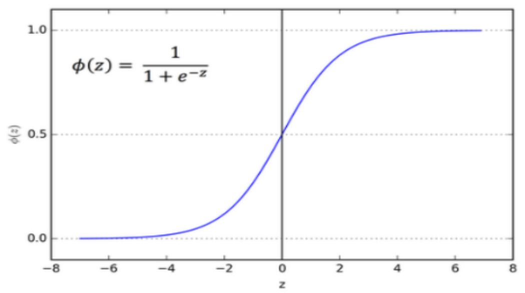
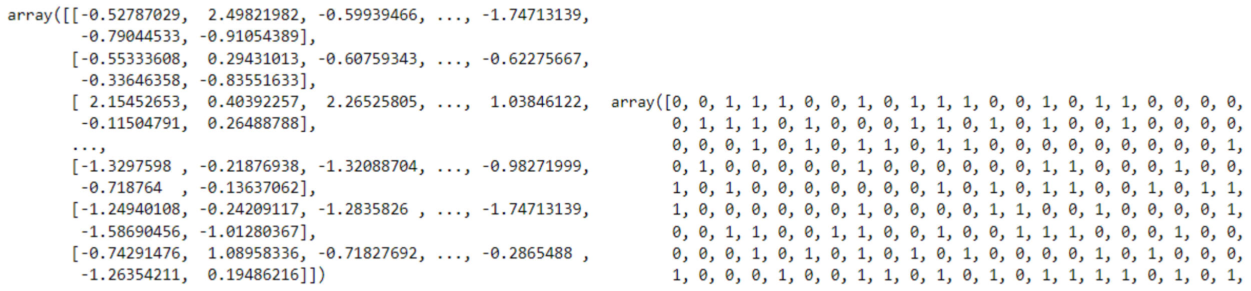


Fig: (Top Right) Dataset; Fig: (Bottom Left) Sigmoid Activation Function ; Fig: (Left) Dataset Column Datatypes

The next step is we perform data preprocessing. We perform the following steps before we can be certain that we can apply the classifier model. This is almost like all the techniques we apply. First, we check for missing data, then check for the spread of the data like where the Mean, Median of the data, are there any outliers, and we take care of that.

In this dataset, there were null values. After that, we label encoded the Diagnosis column to 0 and 1 i.e., whether the patient does not have cancer or do they. After that, I scaled the Train and Test data separately to remove any chance of complications using StandardScalar. The Train and Test split was 80:20.

Below are the X-train set and Y-train set from Left to Right –



```
array([[-0.52787029,  2.49821982, -0.59939466, ..., -1.74713139,
        -0.79044533, -0.91054389],
       [-0.55333608,  0.29431013, -0.60759343, ..., -0.62275667,
        -0.33646358, -0.83551633],
       [ 2.15452653,  0.40392257,  2.26525805, ...,  1.03846122,
        -0.11504791,  0.26488788],
       ...,
       [-1.3297598 , -0.21876938, -1.32088704, ..., -0.98271999,
        -0.718764  , -0.13637062],
       [-1.24940108, -0.24209117, -1.2835826 , ..., -1.74713139,
        -1.58690456, -1.01280367],
       [-0.74291476,  1.08958336, -0.71827692, ..., -0.2865488 ,
        -1.26354211,  0.19486216]])
```

```
array([0, 0, 1, 1, 1, 0, 0, 1, 0, 1, 1, 1, 0, 0, 1, 0, 1, 1, 0, 0, 0, 0,
       0, 1, 1, 1, 0, 1, 0, 0, 0, 1, 1, 0, 1, 0, 1, 0, 0, 1, 0, 0, 0, 0,
       0, 0, 0, 1, 0, 1, 0, 1, 1, 0, 1, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1,
       0, 1, 0, 0, 0, 0, 0, 1, 0, 0, 0, 0, 0, 0, 1, 1, 0, 0, 0, 1, 0, 0,
       1, 0, 1, 0, 0, 0, 0, 0, 0, 1, 0, 1, 0, 1, 1, 0, 0, 1, 0, 1, 1,
       1, 0, 0, 0, 0, 0, 0, 1, 0, 0, 0, 0, 1, 1, 0, 0, 1, 0, 0, 0, 0, 1,
       0, 0, 1, 1, 0, 0, 1, 1, 0, 0, 1, 0, 0, 1, 1, 1, 0, 0, 0, 1, 0, 0,
       0, 0, 0, 1, 0, 1, 0, 1, 0, 1, 0, 1, 0, 0, 0, 0, 1, 0, 1, 0, 0, 0,
       1, 0, 0, 0, 1, 0, 0, 1, 1, 0, 1, 0, 1, 0, 1, 1, 1, 1, 0, 1, 0, 1,
```

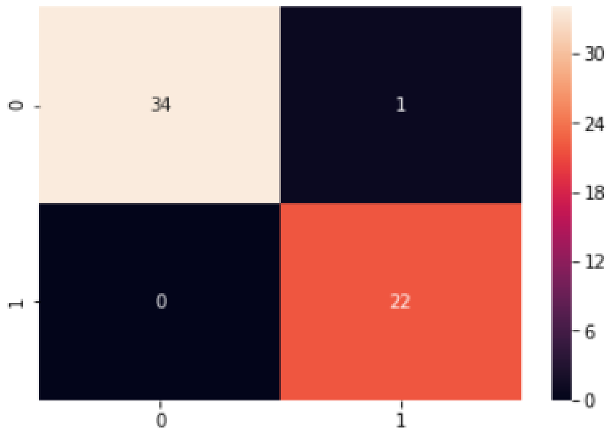
Fig: X-train set, and Y-train set (from Left to Right)

Now we implement the Neural network model on the Training set.

4 Analysis

We find out firstly, the model accuracy for on Test dataset is 98%, which is good considering the data was so complicated. The below confusion matrix depicts that for the most part the prediction for Diagnosis i.e., (M = malignant, B = benign) is done correctly.

Except for one case where the model predicted, a False negative, which means the patient had cancer, but the model predicted they did not. Since the overall prediction is extremely accurate, we can work with this model in the future for new test data.



References

[1] Gareth James [at], Daniela Witten [aut], Trevor Hastie [aut, cre], Rob Tibshirani [aut], Balasubramanian Narasimhan [ctb], *Introduction to Statistical Learning, Second Edition*.

[2] Tom M. Mitchell, *Machine Learning: A multistrategy approach, 1997 Edition*.

[3] Breast Cancer Data: URL - https://archive.ics.uci.edu/ml/datasets/Breast+Cancer+Wisconsin+%28Diagnostic%29