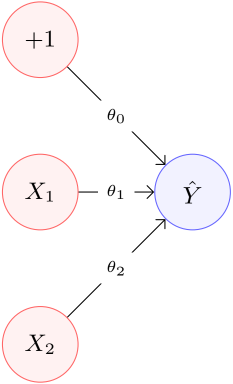
Artificial Neural Networks

Linda Mawhinney

Logistic Regression



$$X = \begin{bmatrix} 1 & x_{1,1} & x_{1,2} \\ \vdots & \vdots & \vdots \\ 1 & x_{m,1} & x_{m,2} \end{bmatrix} \in \mathbb{R}^{m \times 3}$$

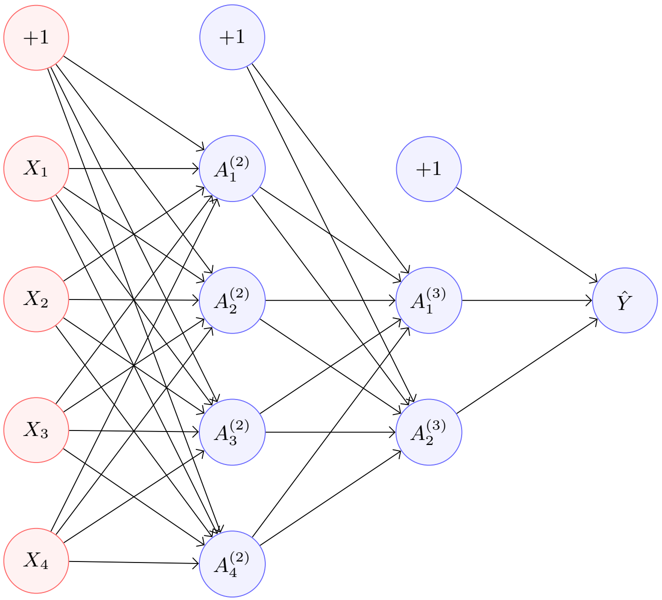
$$\theta = \begin{bmatrix} \theta_0 \\ \theta_1 \\ \theta_2 \end{bmatrix} \in \mathbb{R}^3$$

$$\hat{Y} = \sigma(X\theta) \in [0,1]^m$$

where $\sigma(z) = \frac{1}{1+e^{-z}}$

Cost function:
$J(\theta) = \sum \left(y \log(\hat{y}) + (1-y) \log(1-\hat{y}) \right)$

Hierarchy of Logistic Regressions



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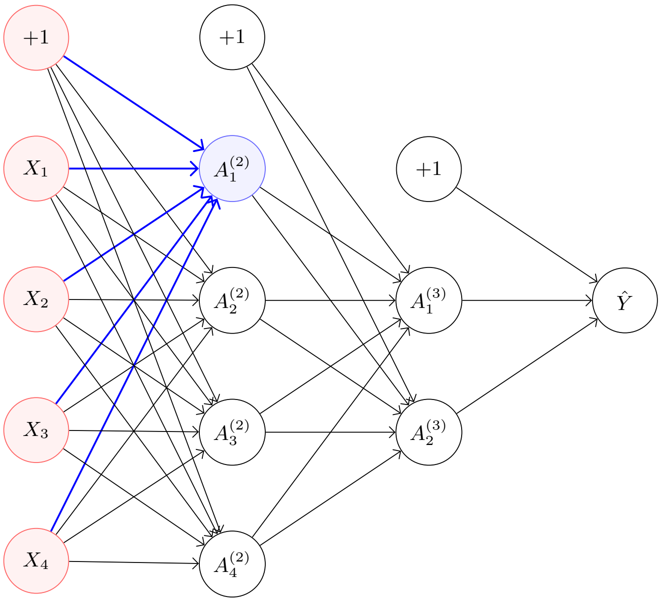
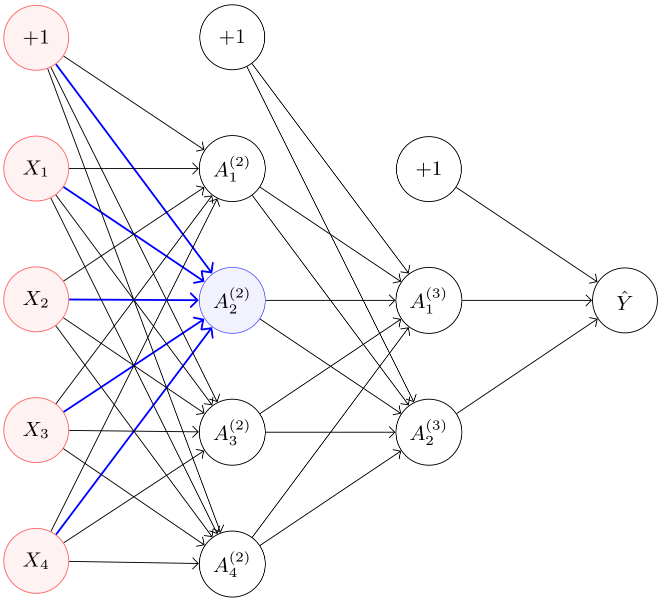


Hierarchy of Logistic Regressions



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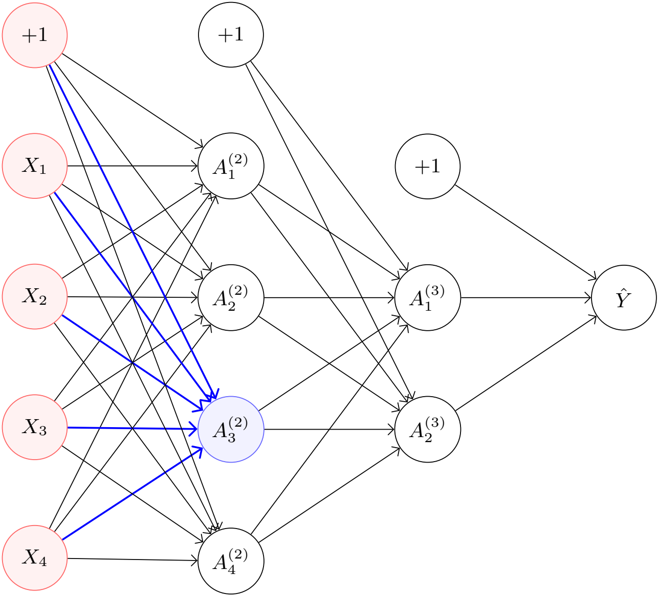

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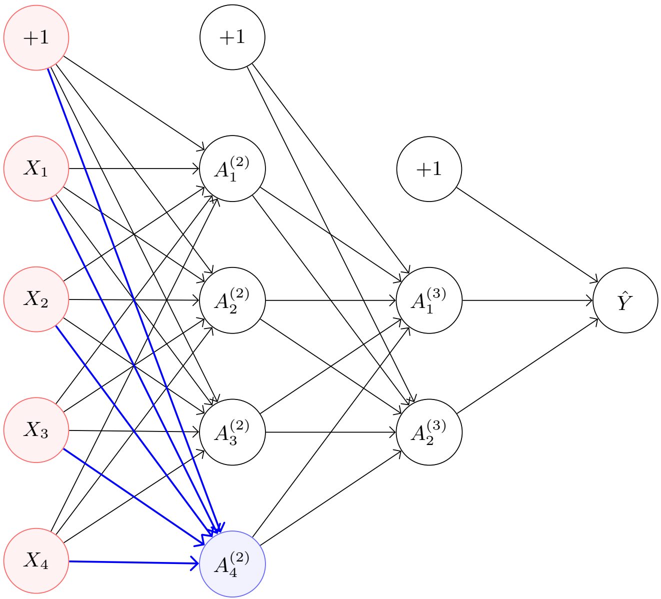

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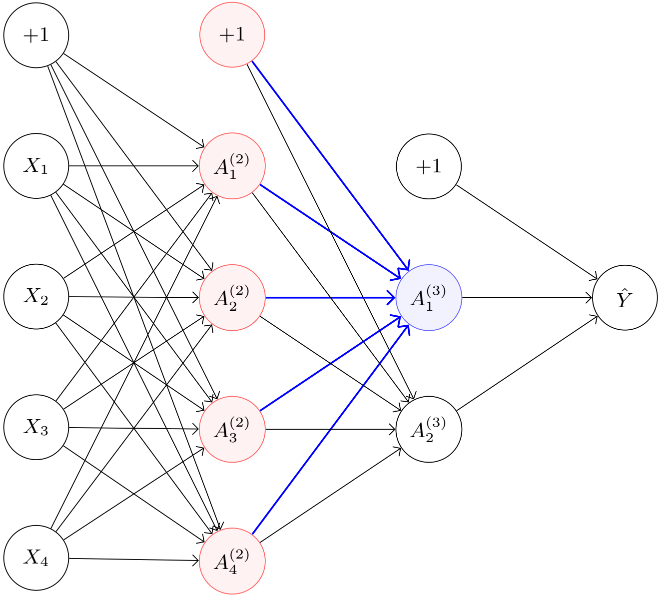

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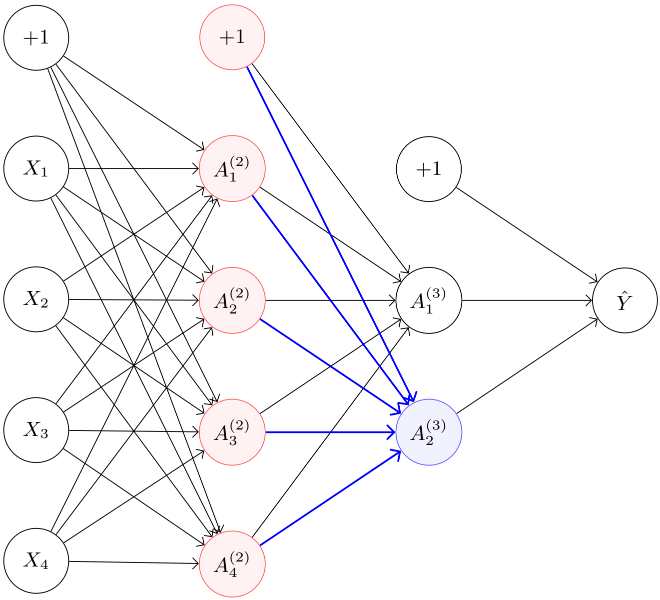

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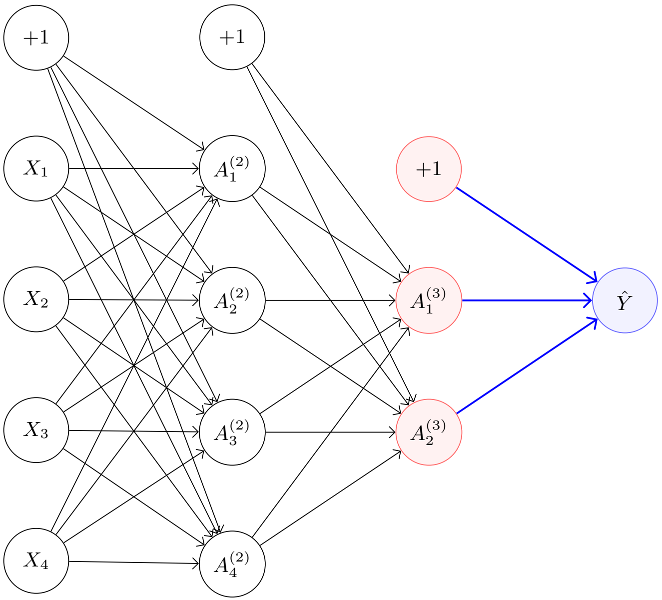
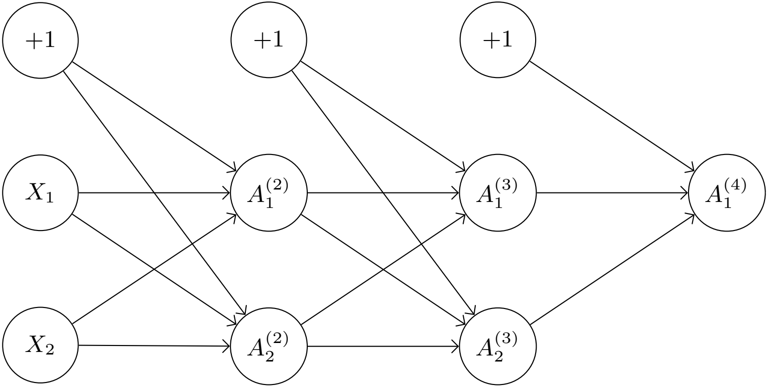
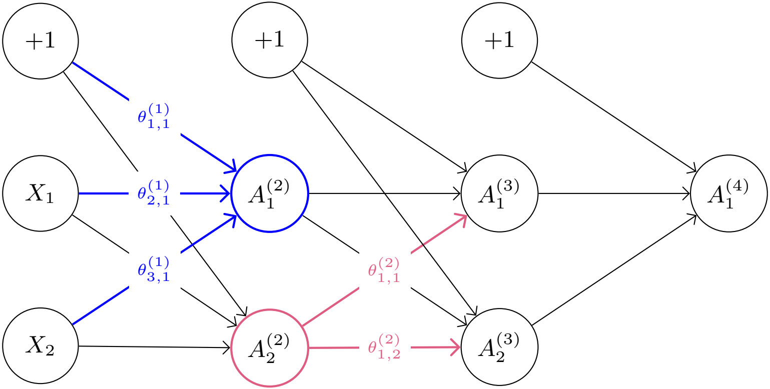


Learning

Algorithm: 2 Hidden Layers, 2 Hidden Nodes



Step 1. Initialize Weights



$$\theta^{(1)} = \begin{bmatrix} \theta_{1,1}^{(1)} & \theta_{1,2}^{(1)} \\ \theta_{2,1}^{(1)} & \theta_{2,2}^{(1)} \\ \theta_{3,1}^{(1)} & \theta_{3,2}^{(1)} \end{bmatrix}, \quad \theta^{(2)} = \begin{bmatrix} \theta_{1,1}^{(2)} & \theta_{1,2}^{(2)} \\ \theta_{2,1}^{(2)} & \theta_{2,2}^{(2)} \\ \theta_{3,1}^{(2)} & \theta_{3,2}^{(2)} \end{bmatrix}, \quad \theta^{(3)} = \begin{bmatrix} \theta_{1,1}^{(3)} \\ \theta_{2,1}^{(3)} \\ \theta_{3,1}^{(3)} \end{bmatrix}$$

Step 2. Feed Forward

- $A^{(1)} \leftarrow \begin{bmatrix} 1 & X \end{bmatrix}$
  $Z^{(2)} = A^{(1)}\theta^{(1)}$
  $A^{(2)} = \sigma(Z^{(2)})$
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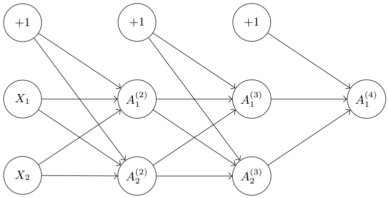
  $Z^{(4)} = A^{(3)}\theta^{(3)}$
  $A^{(4)} = \sigma(Z^{(4)})$



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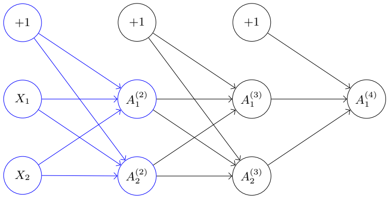

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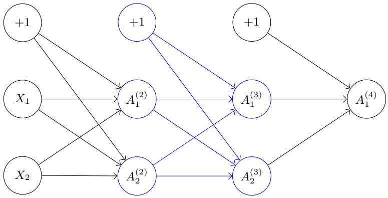

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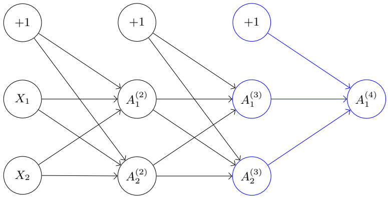
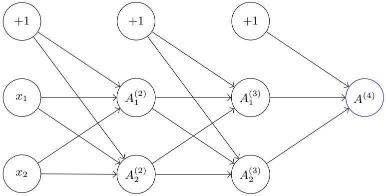


Step 3. Back Propagation

- $\delta^{(4)} = A^{(4)} - Y$
- $\delta^{(3)} = \left(\delta^{(4)}\dot{\theta}^{(3)\top}\right) * \sigma'(Z^{(3)})$
- $\delta^{(2)} = \left(\delta^{(3)}\dot{\theta}^{(2)\top}\right) * \sigma'(Z^{(2)})$



where $\dot{\theta}^{(j)}$ is all but first row of $\theta^{(j)}$, $*$ is the entry-wise product and $\sigma'(z)$ $= \sigma(z)(1 - \sigma(z))$.

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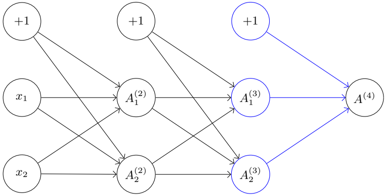

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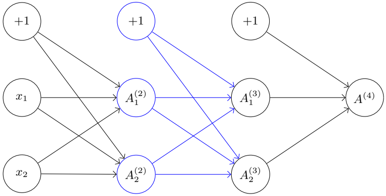

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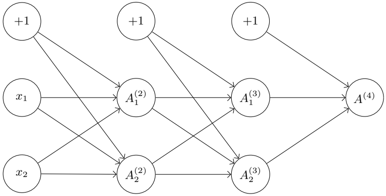


where $\dot{\theta}^{(j)}$ is all but first row of $\theta^{(j)}$, $*$ is the entry-wise product and $\sigma'(z) = \sigma(z)(1 - \sigma(z))$.

$$\frac{\partial J}{\partial \theta^{(1)}} = A^{(1)\top}\delta^{(2)}$$

$$\frac{\partial J}{\partial \theta^{(2)}} = A^{(2)\top}\delta^{(3)}$$

$$\frac{\partial J}{\partial \theta^{(3)}} = A^{(3)\top}\delta^{(4)}$$

Coding in R

R Code

```
initialize.weights <- function(n.hidden.nodes,
                               n.hidden.layers,
                               n.in.nodes,
                               n.out.nodes) {

  W <- list()

  W[[1]] <- random.normal.matrix(n.in.nodes+1, n.hidden.nodes)

  W[[n.hidden.layers+1]] <- random.normal.matrix(n.hidden.nodes+1, n.out.nodes)

  if (n.hidden.layers > 1){
    for (i in 2:n.hidden.layers) {
      W[[i]] <- random.normal.matrix(n.hidden.nodes+1, n.hidden.nodes)
      }
    }

  W

}
```

R Code

```
feed.forward <- function(W, X){

  n.hidden.layers <- length(W) - 1

  A <- list(add.bias.column(X))

  Z <- list(NULL)

  for(i in 1:n.hidden.layers){
    Z[[i+1]] <- A[[i]] %*% W[[i]]
    A[[i+1]] <- add.bias.column(sigmoid(Z[[i+1]]))
  }

  Z[[n.hidden.layers+2]] <- A[[n.hidden.layers+1]] %*% W[[n.hidden.layers+1]]

  A[[n.hidden.layers+2]] <- sigmoid(Z[[n.hidden.layers+2]])

  list(A=A, Z=Z)

}
```

R Code

```
back.prop <- function(A,
                      W,
                      Z,
                      y,
                      n.hidden.layers) {

  delta <- list()

  D <- list()

  delta[[n.hidden.layers+2]] <- A[[n.hidden.layers+2]] - y

  if (n.hidden.layers >= 1){

    for (i in (n.hidden.layers+1):2){
      delta[[i]] <- (delta[[i+1]] %*% t(submatrix(W[[i]], 2))) * sigmoid.grad(Z[[i]])
    }

    for (i in 1:(n.hidden.layers+1)){
      D[[i]] <- t(A[[i]]) %*% delta[[i+1]]
    }

  }

  D

}
```

R Code

```
nn <- function(train.X,
               train.y,
               n.hidden.layers,
               n.hidden.nodes,
               alpha=0.0001,
               tolerance=0.0000001,
               maxiter=1000000) {

  unroll.y <- unroll.matrix(train.y)

  n.in.nodes <- ncol(train.X)
  n.out.nodes <- ncol(unroll.y)
  n <- nrow(train.X)

  W <- initialize.weights(n.hidden.nodes, n.hidden.layers, n.in.nodes, n.out.nodes)

  new <- feed.forward(W, train.X)
  A <- new$A
  Z <- new$Z

  loss <- log.loss(A[[n.hidden.layers+2]], unroll.y)
```

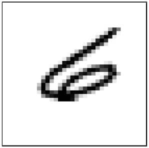
R Code

```
  num.iterations <- 0
  converged <- FALSE

  while (!converged  && num.iterations <  maxiter) {

    num.iterations <- num.iterations + 1

    D <- back.prop(A, W, Z, unroll.y, n.hidden.layers)

    for (i in 1:(n.hidden.layers+1)) {
      W[[i]] <- W[[i]] - alpha * D[[i]]
    }

    new <- feed.forward(W, train.X)
    A <- new$A
    Z <- new$Z

    new.loss <- log.loss(A[[n.hidden.layers+2]], unroll.y)
    converged <- abs((new.loss - loss)/loss) < tolerance
    loss <- new.loss

  }

  list(W=W, iterations=num.iterations, loss=loss)

}
```

Classifying Handwritten Digits

MNIST data set: Classifying hand written digits

Data from images of hand-drawn digits from zero through nine.



$\leftarrow$ 28 pixels $\rightarrow$

- Each image is 784 pixels in total.
- Each pixel has a single pixel-value associated to it.
- Higher numbers mean darker.
- The pixel value is an integer between 0 and 225 inclusive.

MNIST data set

Visually, the pixels make up the image as follows:

$$\begin{array}{cccccc} 000 & 001 & 002 & 003 & \cdots & 027 \\ 028 & 029 & 030 & 031 & \cdots & 055 \\ 056 & 057 & 058 & 059 & \cdots & 083 \\ \vdots & \vdots & \vdots & \vdots & \ldots & \vdots \\ 728 & 729 & 730 & 731 & \cdots & 755 \\ 756 & 757 & 758 & 759 & \cdots & 783 \end{array}$$

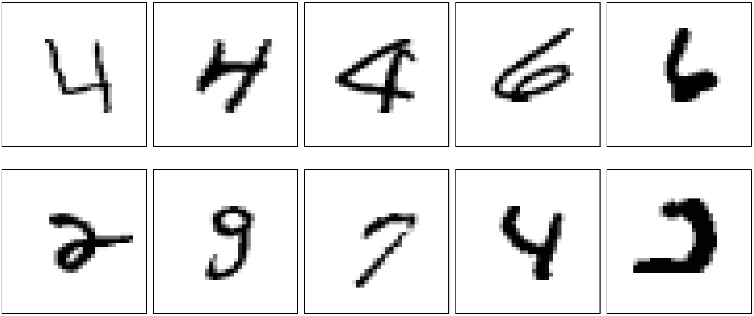
12,000 images

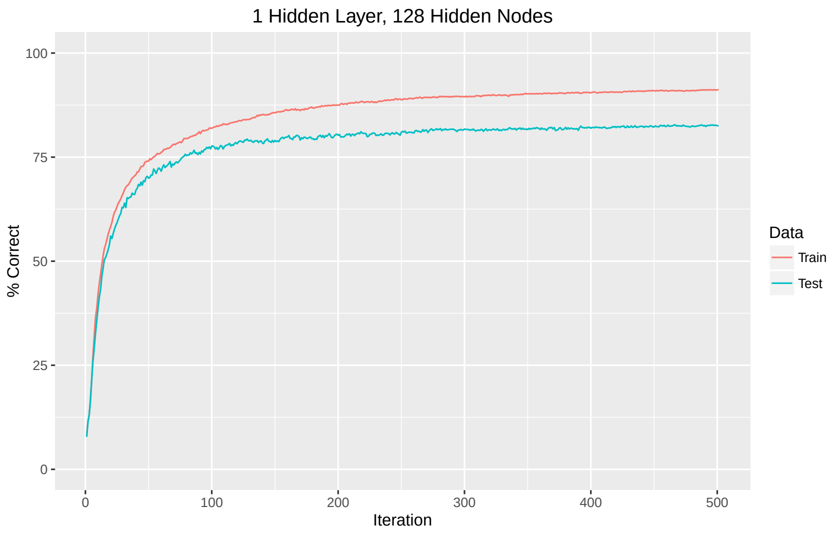
- 10,000 train
- 2,000 test

784 columns

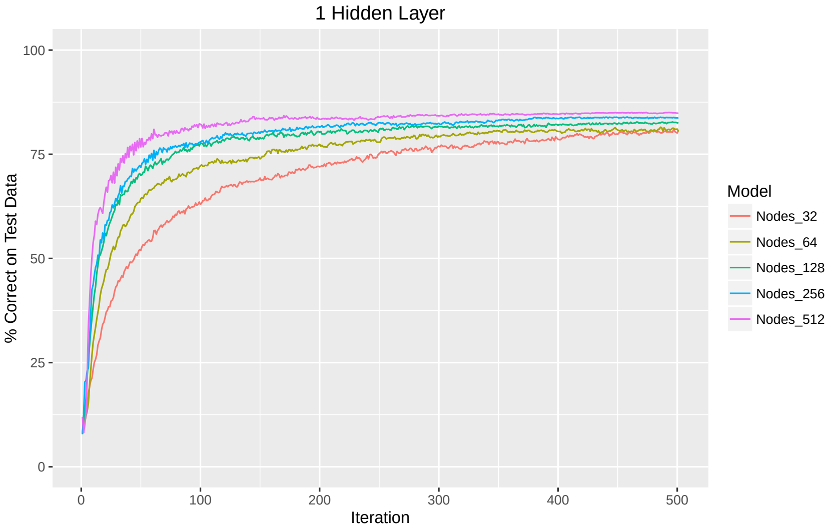
- Pixel 0 - Pixel 783
- Pixel-value

Examples

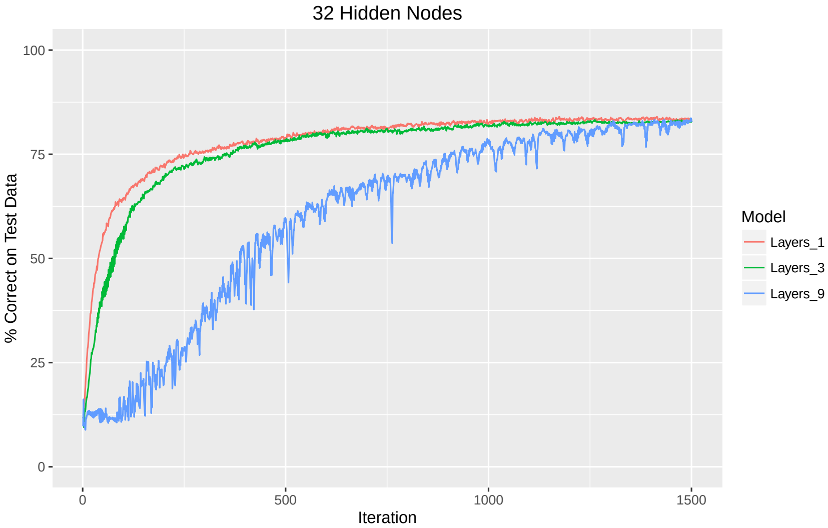


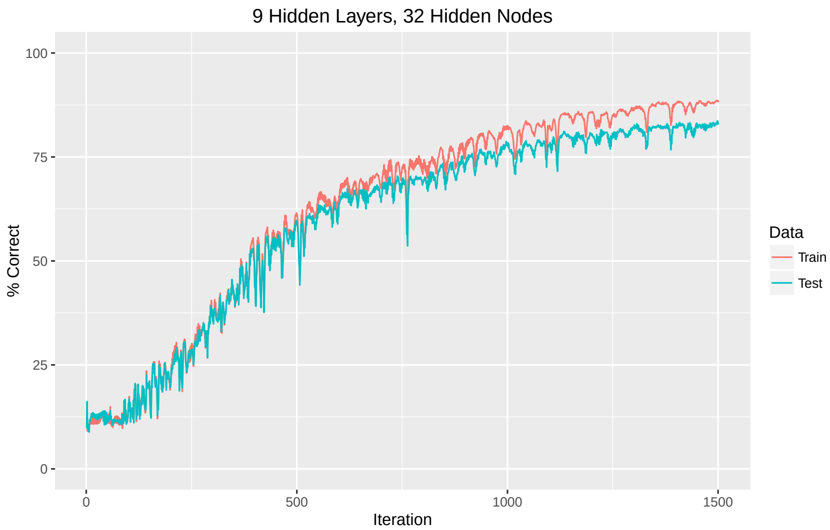


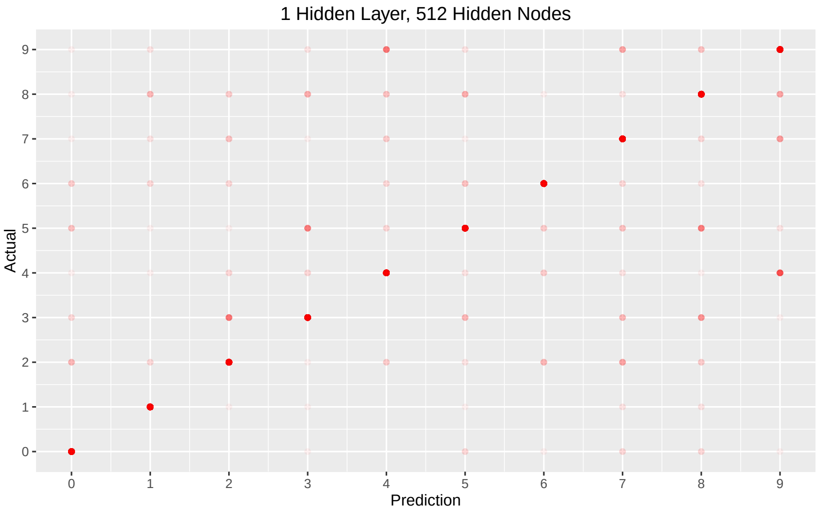
1 Hidden Layer, 128 Hidden Nodes
% Correct
100
75
50
25
0
0
100
200
300
400
500
Iteration
Data
Train
Test



1 Hidden Layer
% Correct on Test Data
100
75
50
25
0
0
100
200
300
400
500
Iteration
Model
Nodes_32
Nodes_64
Nodes_128
Nodes_256
Nodes_512


32 Hidden Nodes
% Correct on Test Data
Iteration
100
75
50
25
0
0
500
1000
1500
Model
Layers_1
Layers_3
Layers_9


9 Hidden Layers, 32 Hidden Nodes
% Correct
100
75
50
25
0
0
500
1000
1500
Iteration
Data
Train
Test

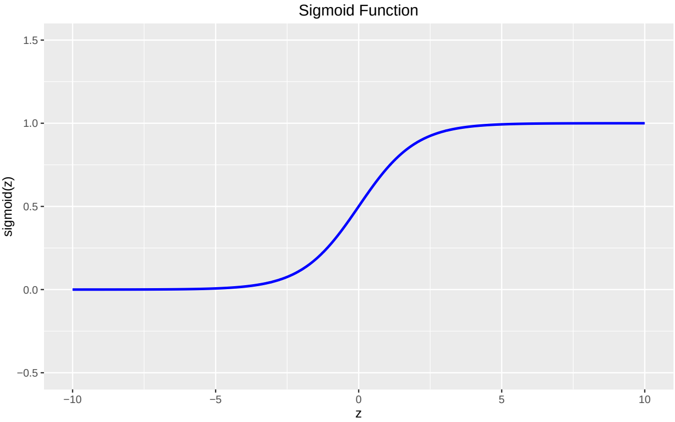


1 Hidden Layer, 512 Hidden Nodes
Actual
Prediction
0
1
2
3
4
5
6
7
8
9

More on Neural Networks

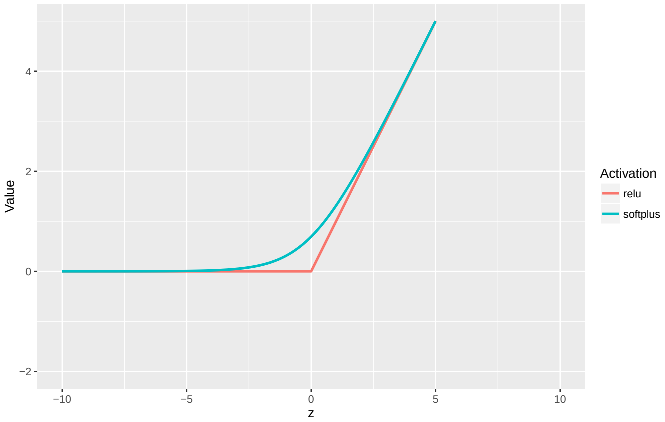
Activation Functions

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



Activation Functions

$$\mathrm{ReLU}(z) = \max(z, 0)$$
$$\mathrm{softplus}(z) = \ln(1 + e^z)$$



Some Issues in Training Neural Networks

- Symmetry breaking
- Chosing architecture
- Overfitting
- Error function is non-convex

References

[1] T. Hastie and R. Tibshirani and J. Freidman, *The Elements of Statistical Learning*, Springer, 2009

[2] A. Ng, *An Introduction to Machine Learning*, Coursera, 2016

[3] Y. LeCun, L. Bottou, Y. Bengio, and P. Haffner. *Gradient-based learning applied to document recognition.* Proceedings of the IEEE, 86(11):2278-2324, November 1998

[4] M. Nielsen, *Neural Networks and Deep Learning*, Determination Press, 2015