

Introduction to Machine Learning

Neural Networks

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Extending Linear Models

Multi Layered Perceptrons

- Generalizing to Multiple Labels

- Properties of Sigmoid Function

- Motivation for Using Non-linear Surfaces

Feed Forward Neural Networks

Backpropagation

- Derivation of the Backpropagation Rules

Final Algorithm

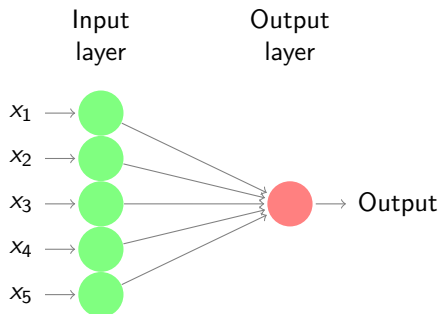
Wrapping up Neural Networks

Bias Variance Tradeoff

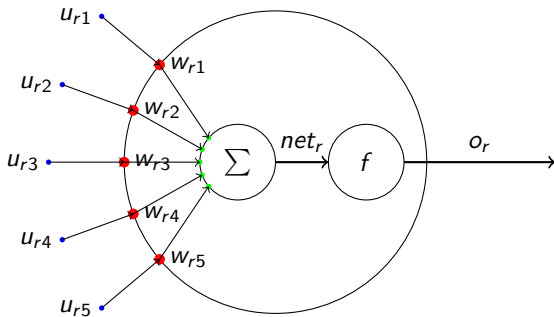
Extending Linear Models

► Questions?

- How to learn non-linear surfaces?
- How to generalize to multiple outputs, numeric output?



Anatomy of a Unit (r)

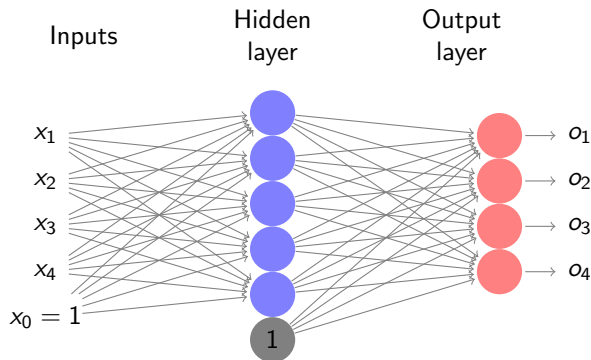


Generalizing to Multiple Labels

- ▶ Distinguishing between multiple categories
- ▶ *Solution:* Add another layer - **Multi Layer Neural Networks**

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What Activation Unit to Use?

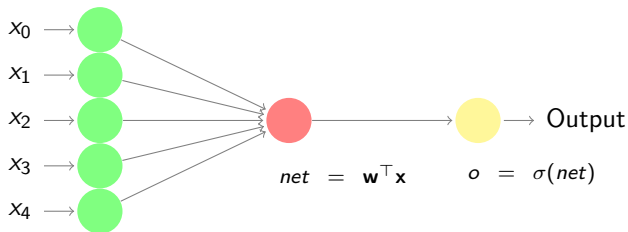
- ▶ Linear Unit
- ▶ Perceptron Unit

What Activation Unit to Use?

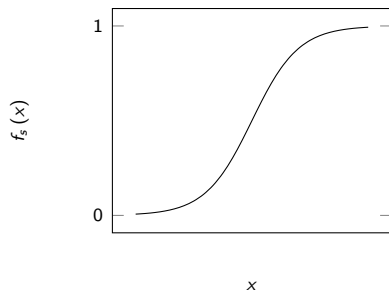
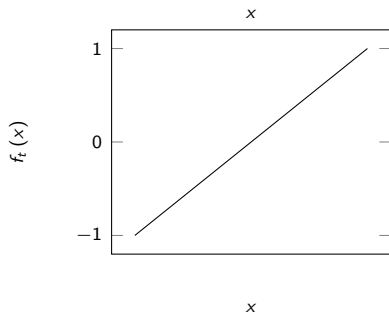
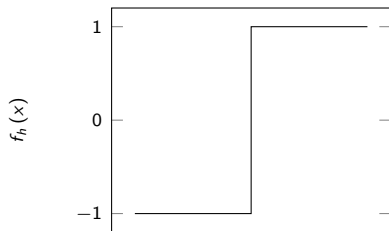
- ▶ Linear Unit
- ▶ Perceptron Unit
- ▶ Sigmoid Unit
 - ▶ Smooth, differentiable activation function

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

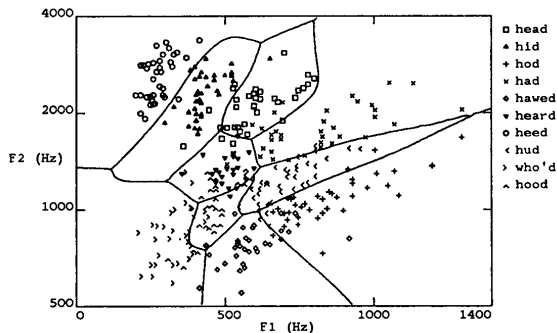
- ▶ Non-linear output



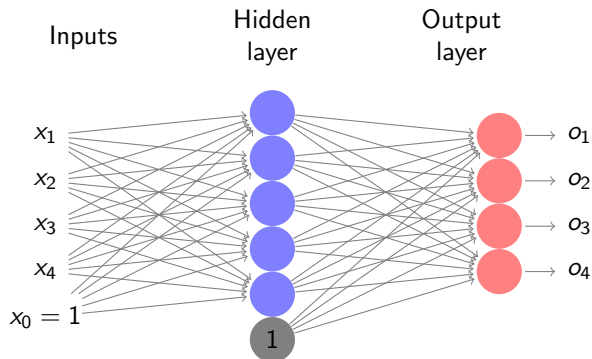
Properties of Sigmoid Function



Motivation for Using Non-linear Surfaces



Feed Forward Neural Networks - Architecture



Feed Forward Neural Networks

- ▶ D input nodes (excluding bias)
 - ▶ M hidden nodes (excluding bias)
 - ▶ K output nodes
- ▶ At hidden nodes: $\mathbf{w}_j, 1 \leq j \leq M, \mathbf{w}_j \in \mathbb{R}^{D+1}$
 - ▶ At output nodes: $\mathbf{w}_l, 1 \leq l \leq K, \mathbf{w}_l \in \mathbb{R}^{M+1}$

Learning Weights of the Multi-layer Network

- ▶ Assume that the network structure is predetermined (number of hidden nodes and interconnections)
- ▶ Objective function for N training examples:

$$J = \sum_{i=1}^N J_i = \frac{1}{2} \sum_{i=1}^N \sum_{l=1}^K (y_{il} - o_{il})^2$$

- ▶ y_{il} - Target value associated with l^{th} class for input (\mathbf{x}_i)
- ▶ $y_{il} = 1$ when k is true class for \mathbf{x}_i , and 0 otherwise
- ▶ o_{il} - Predicted output value at l^{th} output node for \mathbf{x}_i

What are we learning?

Weight vectors for all output and hidden nodes that minimize J

The Backpropagation Algorithm

1. Initialize all weights to *small values*
2. For each training example, $\langle \mathbf{x}, \mathbf{y} \rangle$:
 - 2.1 **Propagate input forward** through the network
 - 2.2 **Propagate errors backward** through the network

Backpropagation Algorithm - Continued

Gradient Descent

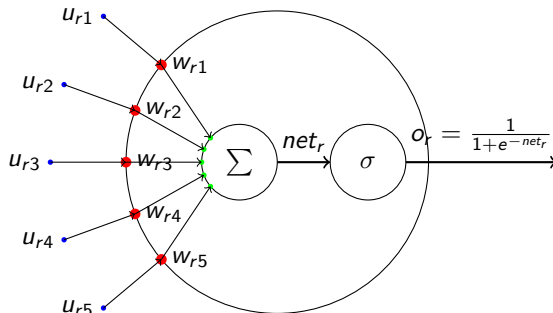
- ▶ Move in the opposite direction of the **gradient** of the objective function
- ▶ $-\eta \nabla J$

$$\nabla J = \sum_{i=1}^N \nabla J_i$$

- ▶ What is the gradient computed with respect to?
 - ▶ Weight vectors - M at hidden nodes and K at output nodes
 - ▶ \mathbf{w}_j ($j = 1 \dots M$)
 - ▶ \mathbf{w}_l ($l = 1 \dots K$)
- ▶ $\mathbf{w}_j \leftarrow \mathbf{w}_j - \eta \frac{\partial J}{\partial \mathbf{w}_j} = \mathbf{w}_j - \eta \sum_{i=1}^N \frac{\partial J_i}{\partial \mathbf{w}_j}$
- ▶ $\mathbf{w}_l \leftarrow \mathbf{w}_l - \eta \frac{\partial J}{\partial \mathbf{w}_l} = \mathbf{w}_l - \eta \sum_{i=1}^N \frac{\partial J_i}{\partial \mathbf{w}_l}$

$$\nabla J_i = \begin{bmatrix} \frac{\partial J_i}{\partial \mathbf{w}_1} \\ \frac{\partial J_i}{\partial \mathbf{w}_2} \\ \vdots \\ \frac{\partial J_i}{\partial \mathbf{w}_{m+k}} \end{bmatrix}$$

Anatomy of a Sigmoid Unit (r)



$$\frac{\partial J_i}{\partial \mathbf{w}_r} = \begin{bmatrix} \frac{\partial J_i}{\partial w_{r1}} \\ \frac{\partial J_i}{\partial w_{r2}} \\ \vdots \end{bmatrix}$$

- ▶ Need to compute $\frac{\partial J_i}{\partial w_{rq}}$
- ▶ Update rule for the q^{th} entry in the r^{th} weight vector:

$$w_{rq} \leftarrow w_{rq} - \eta \frac{\partial J}{\partial w_{rq}} = w_{rq} - \eta \sum_{i=1}^N \frac{\partial J_i}{\partial w_{rq}}$$

Derivation of the Backpropagation Rules

Assume that we only one training example, i.e., $i = 1$, $J = J_i$. Dropping the subscript i from here onwards.

- ▶ Consider any weight w_{rq}
- ▶ Let u_{rq} be the q^{th} element of the input vector coming in to the r^{th} unit.

Observation 1

Weight w_{rq} is connected to J through $net_r = \sum_q w_{rq} u_{rq}$.

$$\frac{\partial J}{\partial w_{rq}} = \frac{\partial J}{\partial net_r} \frac{\partial net_r}{\partial w_{rq}} = \frac{\partial J}{\partial net_r} u_{rq}$$

Analyzing Output Nodes

Observation 2

net_l for an **output node** is connected to J only through the output value of the node (or o_l)

$$\frac{\partial J}{\partial net_l} = \frac{\partial J}{\partial o_l} \frac{\partial o_l}{\partial net_l}$$

Analyzing Output Nodes

Observation 2

net_I for an **output node** is connected to J only through the output value of the node (or o_I)

$$\frac{\partial J}{\partial net_I} = \frac{\partial J}{\partial o_I} \frac{\partial o_I}{\partial net_I}$$

Update Rule for Output Units

$$w_{Ij} \leftarrow w_{Ij} + \eta \delta_I u_{Ij}$$

where $\delta_I = (y_I - o_I)o_I(1 - o_I)$.

► *Question:* What is u_{Ij} for the I^{th} output node?

Observation 3

net_j for a **hidden node** is connected to J through all output nodes

$$\frac{\partial J}{\partial net_j} = \sum_{l=1}^K \frac{\partial J}{\partial net_l} \frac{\partial net_l}{\partial net_j}$$

Analyzing Hidden Nodes

Observation 3

net_j for a **hidden node** is connected to J through all output nodes

$$\frac{\partial J}{\partial net_j} = \sum_{l=1}^K \frac{\partial J}{\partial net_l} \frac{\partial net_l}{\partial net_j}$$

Update Rule for Hidden Units

$$w_{jp} \leftarrow w_{jp} + \eta \delta_j u_{jp}$$

Analyzing Hidden Nodes

Observation 3

net_j for a **hidden node** is connected to J through all output nodes

$$\frac{\partial J}{\partial net_j} = \sum_{l=1}^K \frac{\partial J}{\partial net_l} \frac{\partial net_l}{\partial net_j}$$

Update Rule for Hidden Units

$$w_{jp} \leftarrow w_{jp} + \eta \delta_j u_{jp}$$

$$\delta_j = o_j(1 - o_j) \sum_{l=1}^K \delta_l w_{lj}$$

$$\delta_l = (y_l - o_l) o_l(1 - o_l)$$

- *Question:* What is u_{jp} for the j^{th} hidden node?

Final Algorithm

- ▶ While not converged:
 - ▶ *Move forward* to compute outputs at hidden and output nodes
 - ▶ *Move backward* to propagate errors back
 - ▶ Compute δ errors at output nodes (δ_l)
 - ▶ Compute δ errors at hidden nodes (δ_j)
 - ▶ Update all weights according to weight update equations

Conclusions about Neural Networks

- ▶ Error function contains many local minima
- ▶ No guarantee of convergence
 - ▶ Not a “big” issue in practical deployments
- ▶ Improving backpropagation

Conclusions about Neural Networks

- ▶ Error function contains many local minima
- ▶ No guarantee of convergence
 - ▶ Not a “big” issue in practical deployments
- ▶ Improving backpropagation
 - ▶ Adding momentum
 - ▶ Using stochastic gradient descent
 - ▶ Train multiple times using different initializations

Bias Variance Tradeoff

- ▶ Neural networks are *universal function approximators*
 - ▶ By making the model more complex (increasing number of hidden layers or m) one can lower the error
- ▶ Is the model with least training error the best model?

Bias Variance Tradeoff

- ▶ Neural networks are *universal function approximators*
 - ▶ By making the model more complex (increasing number of hidden layers or m) one can lower the error
- ▶ Is the model with least training error the best model?
 - ▶ The simple answer is **no!**
 - ▶ Risk of overfitting (chasing the data)
 - ▶ Overfitting \Leftarrow **High generalization error**

High Variance - Low Bias

- ▶ “Chases the data”
- ▶ Very low training error
- ▶ Poor performance on unseen data

Low Variance - High Bias

- ▶ Less sensitive to training data
- ▶ Higher training error
- ▶ Better performance on unseen data

Getting the Right Balance

- ▶ General rule of thumb – If two models are giving similar training error, choose the **simpler** model
- ▶ What is simple for a neural network?
- ▶ Low weights in the weight matrices?
 - ▶ Why?

Introducing Bias in Neural Network Training

- ▶ Penalize solutions in which the weights are high
- ▶ Can be done by introducing a penalty term in the objective function
 - ▶ **Regularization**

Regularization for Backpropagation

$$\tilde{J} = J + \frac{\lambda}{2n} \left(\sum_{j=1}^M \sum_{i=1}^{D+1} (w_{ji}^{(1)})^2 + \sum_{l=1}^K \sum_{j=1}^{M+1} (w_{lj}^{(2)})^2 \right)$$

Other Extensions?

- ▶ Use a different loss function (why)?
 - ▶ Quadratic (Squared), Cross-entropy, Exponential, KL Divergence, etc.
- ▶ Use a different activation function (why)?
 - ▶ Sigmoid

$$f(z) = \frac{1}{1 + \exp(-z)}$$

- ▶ Tanh

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

- ▶ Rectified Linear Unit (ReLU)

$$f(z) = \max(0, z)$$

References