Introduction to Machine Learning

Neural Networks

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Outline

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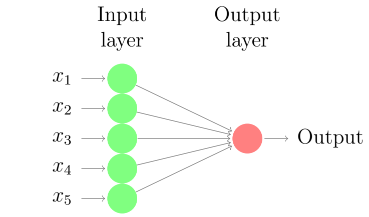
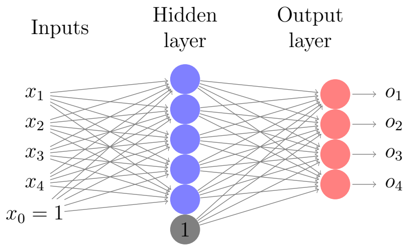
1 Extending Linear Models

- Questions?





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

2 Multi Layered Perceptrons

2.1 Generalizing to Multiple Labels

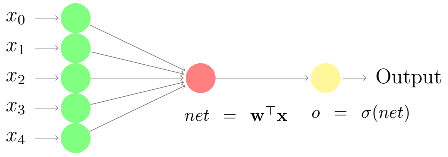
- Distinguishing between multiple categories
- *Solution:* Add another layer - **Multi Layer Neural Networks**

Multi-class classification is more applicable than binary classification. Applications include, handwritten digit recognition, robotics, etc.

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

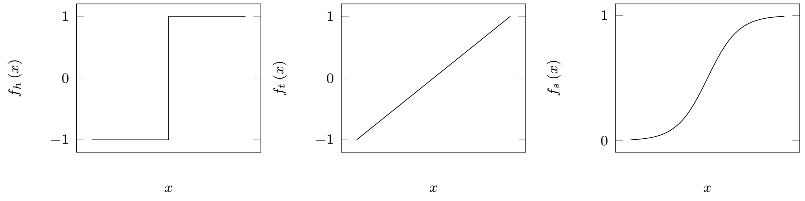
$$\sigma(net) = \frac{1}{1+e^{-net}}$$

  - Non-linear output



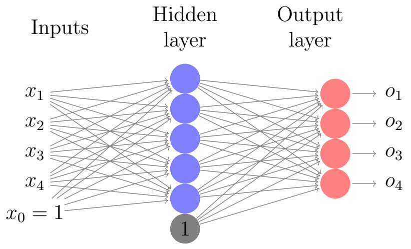
As mentioned earlier, the perceptron unit cannot be used as it is not differentiable. The linear unit is differentiable but only learns linear discriminating surfaces. So to learn non-linear surfaces, we need to use a non-linear unit such as the sigmoid.

2.2 Properties of Sigmoid Function



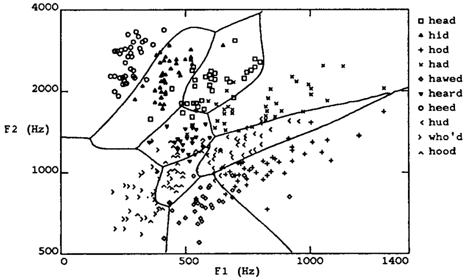
The threshold output in the case of the sigmoid unit is continuous and smooth, as opposed to a perceptron unit or a linear unit. A useful property of sigmoid is that its derivative can be easily expressed as:

$$\frac{D\sigma(y)}{Dy} = \sigma(y)(1-\sigma(y))$$



One can also use e^{-ky} instead of e^{-y}, where k controls the "steepness" of the threshold curve.

2.3 Motivation for Using Non-linear Surfaces



The learning problem is to recognize 10 different vowel sounds from the audio input. The raw sound signal is compressed into two features using spectral analysis.

3 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: $\mathbf{w_l}, 1 \leq l \leq K$, $\mathbf{w_l} \in \mathbb{R}^{M+1}$

The multi-layer neural network shown above is used in a feed forward mode, i.e., information only flows in one direction (forward). Each hidden node "collects" the inputs from all input nodes and computes a weighted sum of the inputs and then applies the sigmoid function to the weighted sum. The output of each hidden node is forwarded to every output node. The output node "collects" the inputs (from hidden layer nodes) and computes a weighted sum of its inputs and then applies the sigmoid function to obtain the final output. The class corresponding to the output node with the largest output value is assigned as the predicted class for the input.

For implementation, one can even represent the weights as two matrices, $W^{(1)}$ $(M \times D+1)$ and $W^{(2)}$ $(K \times M+1)$.

4 Backpropagation

- 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 first question that comes to mind is, why not use a standard gradient descent based minimization as the one that we saw in single perceptron unit learning. The reason is that the output at every output node (o_l) is directly dependent on the weights associated with the output nodes but not with weights at hidden nodes. But the input values are "used" by the hidden nodes and are not "visible" to the output nodes. To learn all the weights simultaneously, direct minimization is not possible. Advanced methods such as **Backpropagation** need to be employed.

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

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
  - $\mathbf{w}_j$ $(j = 1 \ldots M)$
  - $\mathbf{w}_l$ $(l = 1 \ldots K)$
- $\mathbf{w}_j \leftarrow \mathbf{w}_j - \eta \frac{\partial J}{\partial \mathbf{w}_j} = \mathbf{w}_j - \eta \sum_{i=1}^{N} \frac{\partial J_i}{\partial \mathbf{w}_j}$
- $\mathbf{w}_l \leftarrow \mathbf{w}_l - \eta \frac{\partial J}{\partial \mathbf{w}_l} = \mathbf{w}_l - \eta \sum_{i=1}^{N} \frac{\partial J}{\partial \mathbf{w}_l}$

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

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

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

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

4.1 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 $net_r = \sum_q w_{rq}u_{rq}$.

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

Observation 2
net_l for an **output node** is connected to J only through the output value of the node (or o_l)

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

The first term above can be computed as:

$$\frac{\partial J}{\partial o_l} = \frac{\partial}{\partial o_l}\frac{1}{2}\sum_{l=1}^{K}(y_l - o_l)^2$$

The entries in the summation in the right hand side will be non zero only for l. This results in:

$$\begin{aligned} \frac{\partial J}{\partial o_l} &= \frac{\partial}{\partial o_l}\frac{1}{2}(y_l - o_l)^2 \\ &= -(y_l - o_l) \end{aligned}$$

Moreover, the second term in the chain rule above can be computed as:

$$\begin{aligned} \frac{\partial o_l}{\partial net_l} &= \frac{\partial \sigma(net_l)}{\partial net_l} \\ &= o_l(1 - o_l) \end{aligned}$$

The last result arises from the fact o_l is a sigmoid function. Using the above results, one can compute the following.

$$\frac{\partial J}{\partial net_l} = -(y_l - o_l)o_l(1 - o_l)$$

Let

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

Therefore,

$$\frac{\partial J}{\partial net_l} = -\delta_l$$

Finally we can compute the partial derivative of the error with respect to the weight w_{lj} as:

$$\frac{\partial J}{\partial w_{lj}} = -\delta_l u_{lj}$$

Update Rule for Output Units

$$w_{lj} \leftarrow w_{lj} + \eta\delta_l u_{lj}$$

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

- *Question:* What is u_{lj} for the l^{th} output node?
- u_{lj} is the j^{th} input to l^{th} output node, which will be the output coming from the j^{th} hidden node.

Observation 3
net_j for a **hidden node** is connected to J through all output nodes

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

Remember that we have already computed the first term on the right hand side for output nodes:

$$\frac{\partial J}{\partial net_l} = -\delta_l$$

where $\delta_l = (y_l - o_l)o_l(1 - o_l)$. This result gives us:

$$\begin{aligned}
\frac{\partial J}{\partial net_j} &= \sum_{l=1}^{K} -\delta_l \frac{\partial net_l}{\partial net_j}\\
&= \sum_{l=1}^{K} -\delta_l \frac{\partial net_l}{\partial z_j}\frac{\partial z_j}{\partial net_j}\\
&= \sum_{l=1}^{K} -\delta_l w_{lj} \frac{\partial z_j}{\partial net_j}\\
&= \sum_{l=1}^{K} -\delta_l w_{lj} z_j(1 - z_j)\\
&= -z_j(1 - z_j)\sum_{l=1}^{K} \delta_l w_{lj}
\end{aligned}$$

Thus, the gradient becomes:

$$\begin{aligned}
\frac{\partial J}{\partial w_{jp}} &= \frac{\partial J}{\partial net_j} u_{jp}\\
&= -z_j(1 - z_j)(\sum_{l=1}^{K} \delta_l w_{lj}) u_{jp}\\
&= -\delta_j u_{jp}
\end{aligned}$$

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?
- u_{jp} is the p^{th} input to j^{th} hidden node, which will be p^{th} attribute value for the input, i.e., x_p.

5 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

6 Wrapping up 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

Adding momentum to the learning process refers to adding an "inertia" term which tries to keep the current value of a weight value similar to the one taken in the previous round.

7 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"
- Model parameters change significantly when the training data is changed, hence the term high variance.
- 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

- 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?

  - The simple answer to this is that if the weights in the weight vectors at each node are high, the resulting discriminating surface learnt by the neural network will be highly non-linear. If the weights are smaller, the surface will be smoother (and hence simpler).
- Penalize solutions in which the weights are high
- Can be done by introducing a penalty term in the objective function
  - **Regularization**

Regularization for Backpropagation

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

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