What Do
Neural Networks Do?

Multi-layer networks

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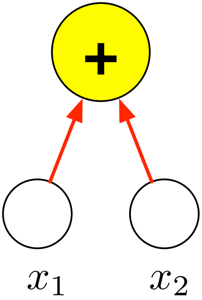
Machine Learning Practical — MLP Lecture 3
5 October 2016

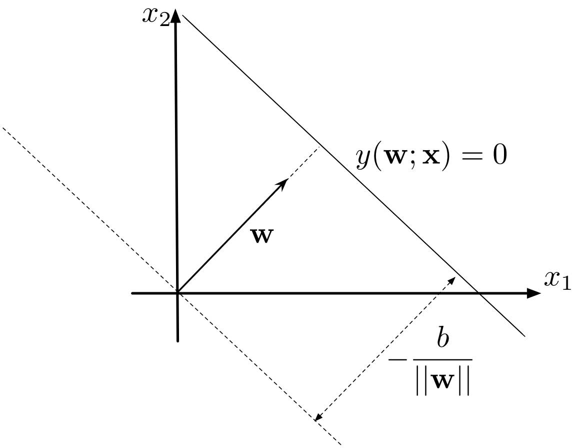
What Do Single Layer Neural Networks Do?

Single layer network

Single-layer network, 1 output, 2 inputs

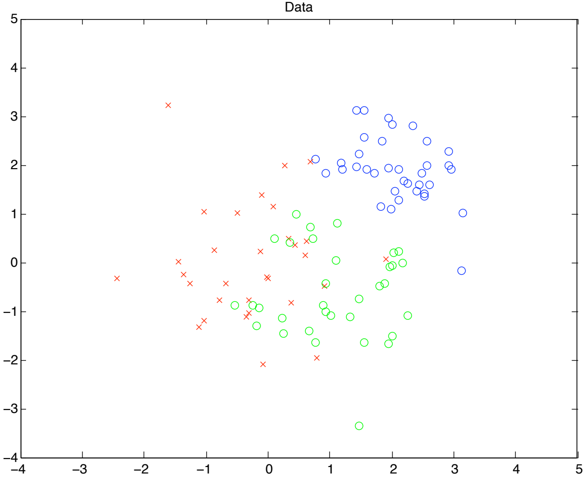


Single-layer network, 1 output, 2 inputs



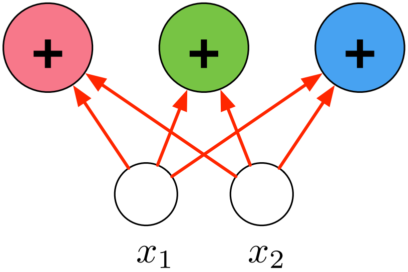
Bishop, sec 3.1

Example data (three classes)

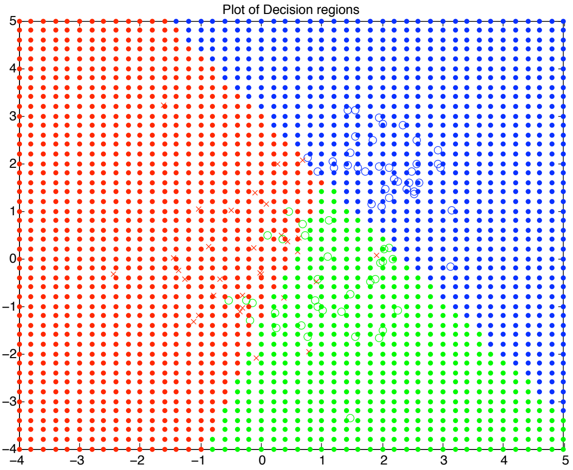


Single layer network

Single-layer network, 3 outputs, 2 inputs

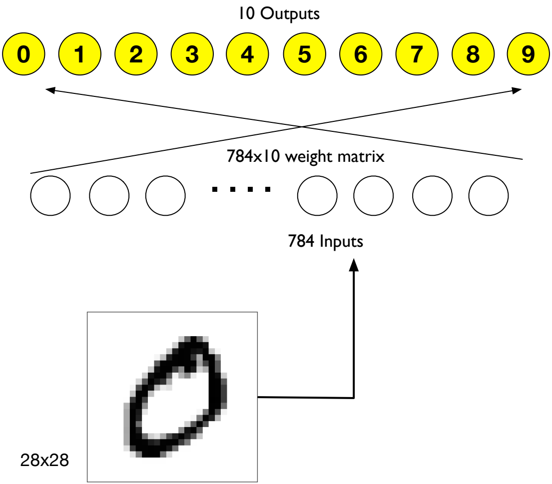


Classification regions with single-layer network



Single-layer networks are limited to linear classification boundaries

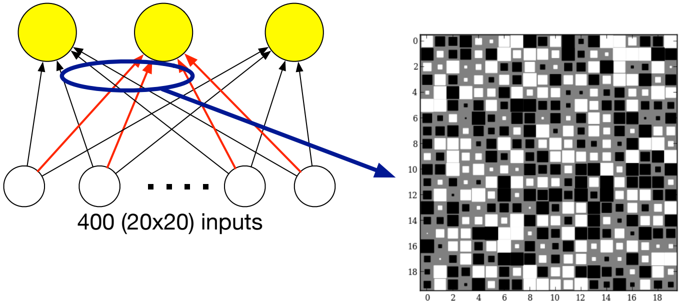
Single layer network trained on MNIST Digits



Output weights define a "template" for each class

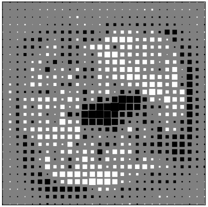
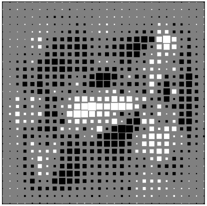
Hinton Diagrams

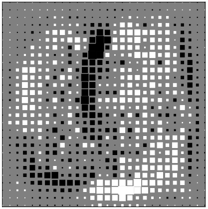
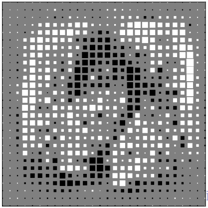
Visualise the weights for class k



Hinton diagram for single layer network trained on MNIST

- Weights for each class act as a "discriminative template"
- Inner product of class weights and input to measure closeness to each template
- Classify to the closest template (maximum value output)

0


1

2


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Multi-Layer Networks

From templates to features

- Good classification needs to cope with the variability of real data: scale, skew, rotation, translation, ...
- Very difficult to do with a single template per class
- Could have multiple templates per task... this will work, but we can do better

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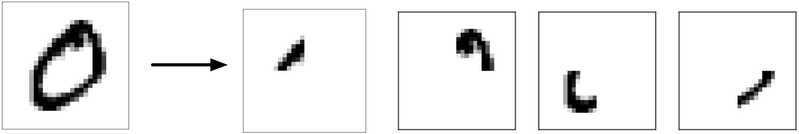
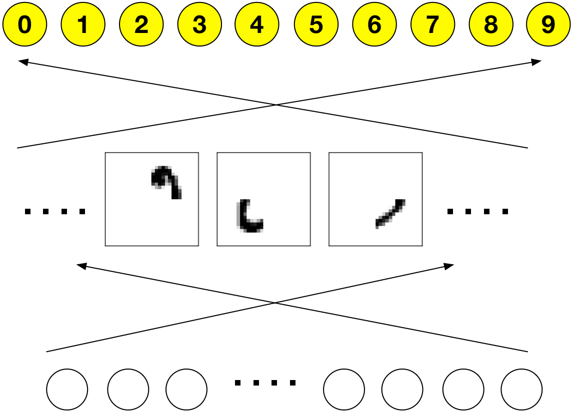
Use features rather than templates



(images from: Michael Nielsen, *Neural Networks and Deep Learning*, http://neuralnetworksanddeeplearning.com/chap1.html)

Incorporating features in neural network architecture

- Layered processing: inputs - features - classification



- How to obtain features - learning!

Incorporating features in neural network architecture

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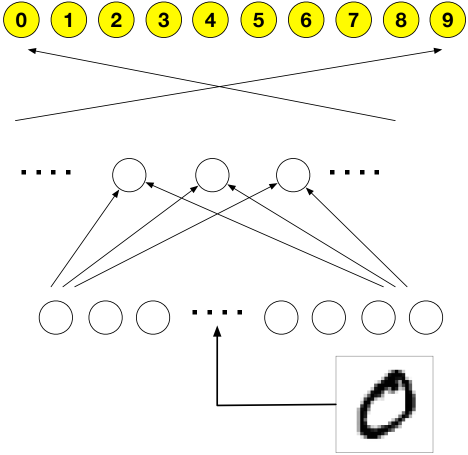

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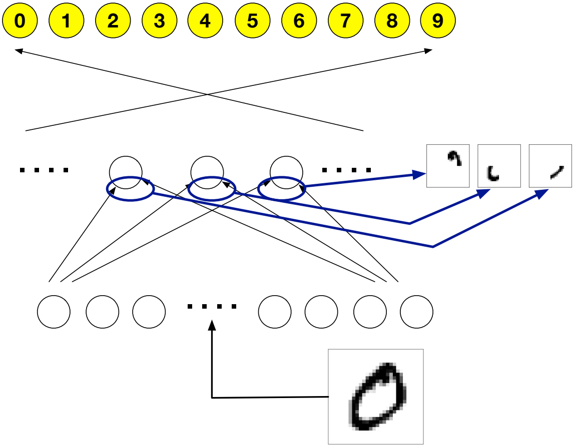

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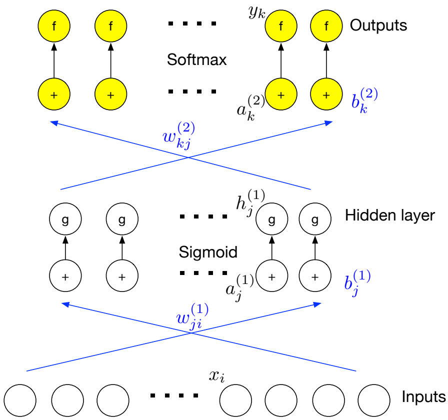
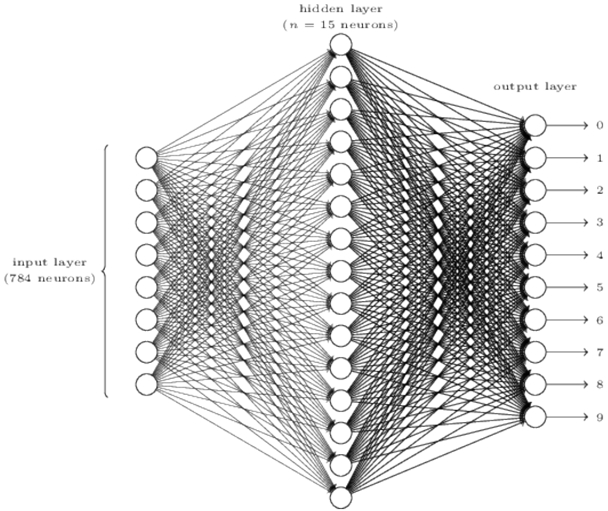
Multi-layer network



$$y_k = \text{softmax}\left(\sum_{r=1}^{H} w_{kr}^{(2)} h_r^{(1)} + b_k\right) \qquad h_j^{(1)} = \text{sigmoid}\left(\sum_{s=1}^{d} w_{js}^{(1)} x_s + b_j\right)$$

Multi-layer network for MNIST

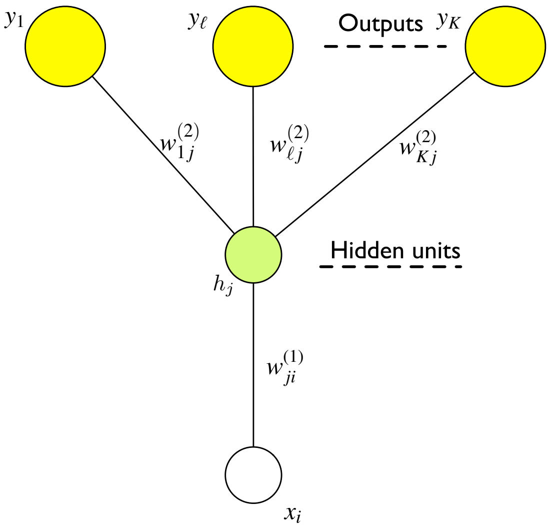


(image from: Michael Nielsen, *Neural Networks and Deep Learning*, http://neuralnetworksanddeeplearning.com/chap1.html)

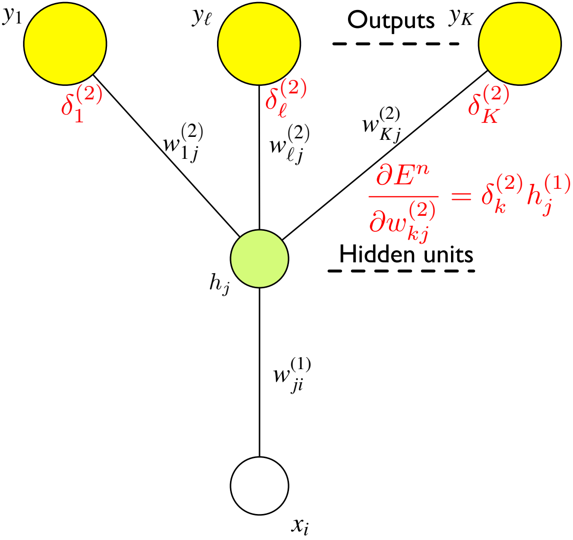
Training MLPs: Credit assignment

- Hidden units make training the weights more complicated, since the hidden units affect the error function indirectly via all the outputs
- The Credit assignment problem: what is the "error" of a hidden unit? how important is input-hidden weight $w_{ji}^{(1)}$ to output unit k?
- Solution: Gradient descent – requires derivatives of the error with respect to each weight
- Algorithm: *back-propagation of error* (backprop)
- Backprop gives a way to compute the derivatives. These derivatives are used by an optimisation algorithm (e.g. gradient descent) to train the weights.

Training output weights



Training output weights



Training MLPs: Error function and required gradients

- Cross-entropy error function:

$$E^n = -\sum_{k=1}^{C} t_k^n \ln y_k^n$$

- Required gradients: $\frac{\partial E^n}{\partial w_{kj}^{(2)}}$ $\frac{\partial E^n}{\partial w_{ji}^{(1)}}$ $\frac{\partial E^n}{\partial b_k^{(2)}}$ $\frac{\partial E^n}{\partial b_j^{(1)}}$
- **Gradient for hidden-to-output weights** similar to single-layer network:

$$\boxed{\frac{\partial E^n}{\partial w_{kj}^{(2)}}} = \frac{\partial E^n}{\partial a_k^{(2)}} \cdot \frac{\partial a_k^{(2)}}{\partial w_{kj}} = \left(\sum_{c=1}^{C} \frac{\partial E^n}{\partial y_c} \cdot \frac{\partial y_c}{\partial a_k^{(2)}} \right) \cdot \frac{\partial a_k^{(2)}}{\partial w_{kj}}$$

$$= \underbrace{(y_k - t_k)}_{\delta_k^{(2)}} h_j^{(1)}$$

Back-propagation of error: hidden unit error signal

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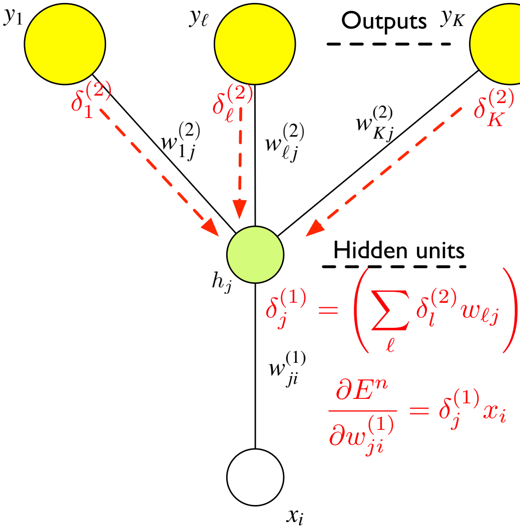


$$\delta_j^{(1)} = \left(\sum_\ell \delta_l^{(2)} w_{\ell j} \right) h_j (1 - h_j)$$

$$\frac{\partial E^n}{\partial w_{ji}^{(1)}} = \delta_j^{(1)} x_i$$

Training MLPs: Input-to-hidden weights

$$\boxed{\frac{\partial E^n}{\partial w_{ji}^{(1)}}} = \underbrace{\frac{\partial E^n}{\partial a_j^{(1)}}}_{\delta_j^{(1)}} \cdot \underbrace{\frac{\partial a_j^{(1)}}{\partial w_{ji}^{(1)}}}_{x_i}$$

To compute $\delta_j^{(1)} = \partial E^n / \partial a_j^{(1)}$, the error signal for hidden unit j, we must sum over all the output units' contributions to $\delta_j^{(1)}$:

$$\boxed{\delta_j^{(1)}} = \sum_{c=1}^{K} \frac{\partial E^n}{\partial a_c^{(2)}} \cdot \frac{\partial a_c^{(2)}}{\partial a_j^{(1)}} = \left(\sum_{c=1}^{K} \delta_c^{(2)} \cdot \frac{\partial a_c^{(2)}}{\partial h_j^{(1)}} \right) \cdot \frac{\partial h_j^{(1)}}{\partial a_j^{(1)}}$$

$$= \left(\sum_{c=1}^{K} \delta_c^{(2)} w_{cj}^{(2)} \right) h_j^{(1)} (1 - h_j^{(1)})$$

Training MLPs: Gradients

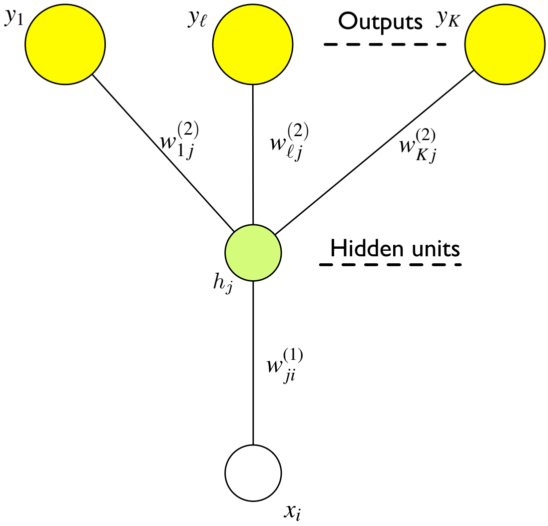
$$\boxed{\frac{\partial E^n}{\partial w_{kj}^{(2)}}} = \underbrace{(y_k - t_k)}_{\delta_k^{(2)}} \cdot h_j^{(1)}$$

$$\boxed{\frac{\partial E^n}{\partial w_{ji}^{(1)}}} = \underbrace{\left(\sum_{c=1}^{k} \delta_c^{(2)} w_{cj}^{(2)}\right) h_j^{(1)}(1 - h_j^{(1)})}_{\delta_j^{(1)}} \cdot x_i$$

- Exercise: write down expressions for the gradients w.r.t. the biases

$$\frac{\partial E^n}{\partial b_k^{(2)}} \qquad \frac{\partial E^n}{\partial b_j^{(1)}}$$

Back-propagation of error: hidden unit error signal



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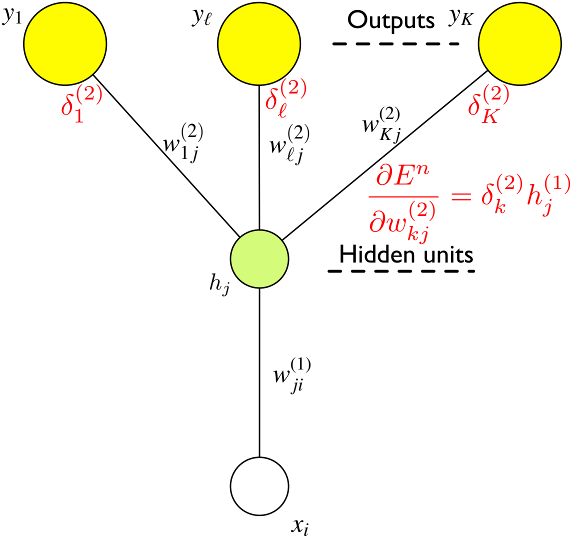

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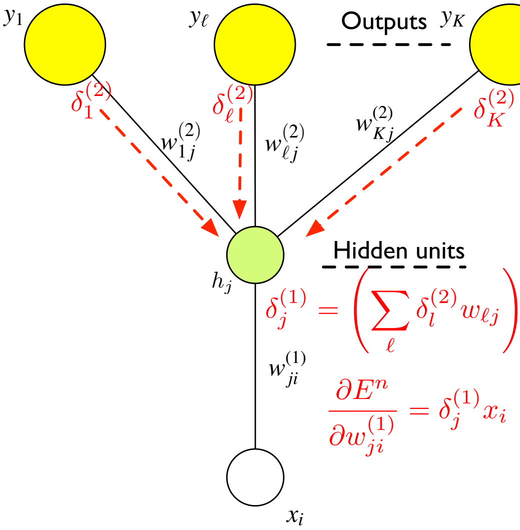


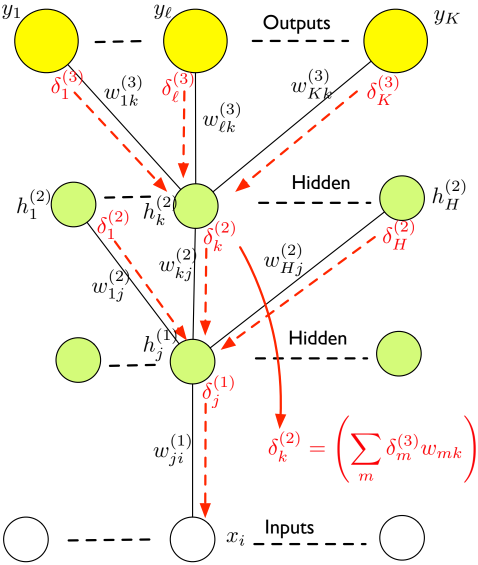
$$\delta_j^{(1)} = \left(\sum_{\ell} \delta_l^{(2)} w_{\ell j} \right) h_j (1 - h_j)$$

$$\frac{\partial E^n}{\partial w_{ji}^{(1)}} = \delta_j^{(1)} x_i$$

Back-propagation of error

- The back-propagation of error algorithm is summarised as follows:
    1. Apply an input vectors from the training set, $\mathbf{x}$, to the network and forward propagate to obtain the output vector $\mathbf{y}$
    2. Using the target vector $\mathbf{t}$ compute the error E^n
    3. Evaluate the error signals $\delta_k^{(2)}$ for each output unit
    4. Evaluate the error signals $\delta_j^{(1)}$ for each hidden unit using back-propagation of error
    5. Evaluate the derivatives for each training pattern
- Back-propagation can be extended to multiple hidden layers, in each case computing the $\delta^{(\ell)}$s for the current layer as a weighted sum of the $\delta^{(\ell+1)}$s of the next layer

Training with multiple hidden layers



$$\delta_k^{(2)} = \left(\sum_m \delta_m^{(3)} w_{mk} \right) h_k^{(2)} (1 - h_k^{(2)})$$

Summary

- Understanding what single-layer networks compute
- How multi-layer networks allow feature computation
- Training multi-layer networks using back-propagation of error
- Reading:
  Michael Nielsen, chapters 1 & 2 of *Neural Networks and Deep Learning*
  http://neuralnetworksanddeeplearning.com/
  Chris Bishop, Sections 3.1, 3.2, and Chapter 4 of *Neural Networks for Pattern Recognition*