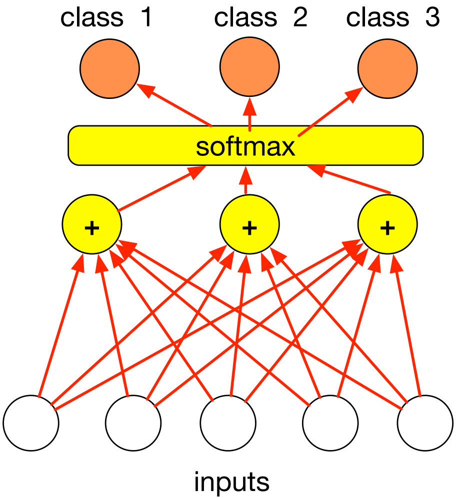
Deep Neural Networks (1)
Hidden layers; Back-propagation

Steve Renals

Machine Learning Practical — MLP Lecture 3
2 October 2018
http://www.inf.ed.ac.uk/teaching/courses/mlp/

Recap: Softmax single layer network



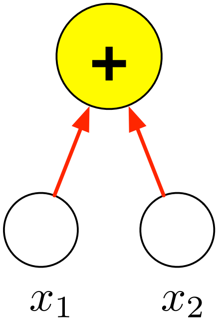
What Do

Neural Networks Do?

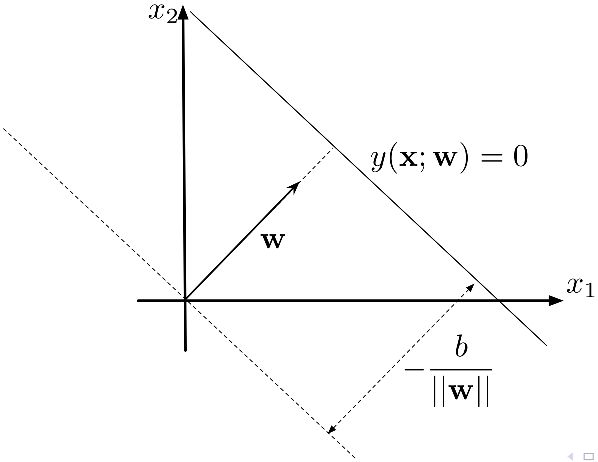
What Do
Single Layer
Neural Networks Do?

Single layer network

Single-layer network, 1 output, 2 inputs

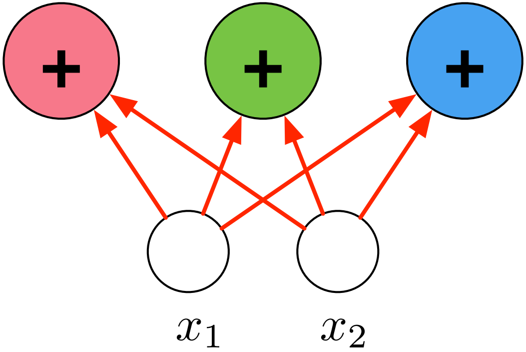


Single-layer network, 1 output, 2 inputs

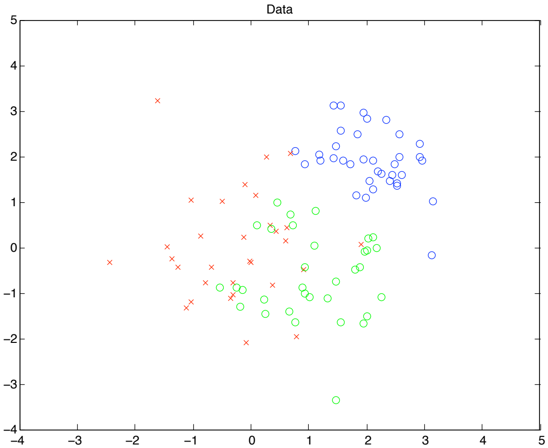


Single layer network

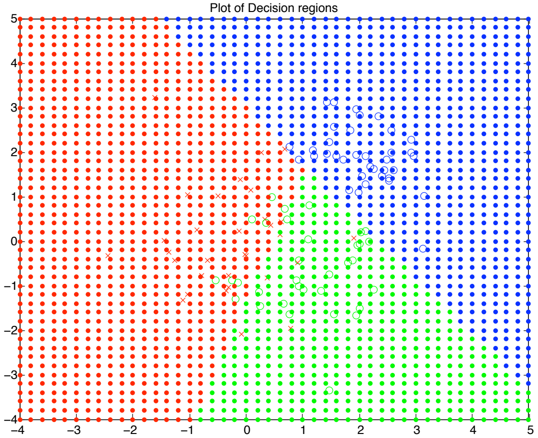
Single-layer network, 3 outputs, 2 inputs



Example data (three classes)

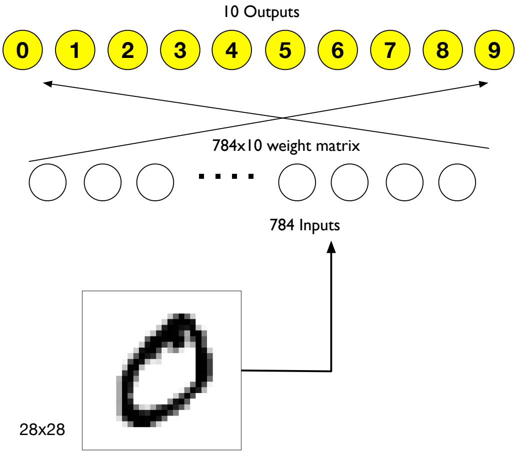


Classification regions with single-layer network



Single-layer networks are limited to linear classification boundaries

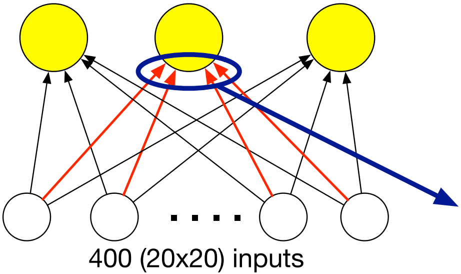
Single layer network trained on MNIST Digits

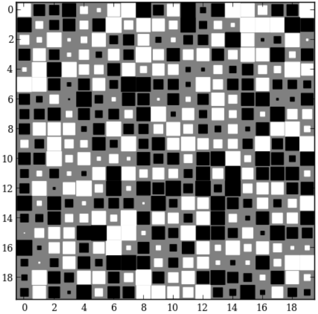


Weights of each output unit define a "template" for the class

Hinton Diagrams

Visualise the weights for class k



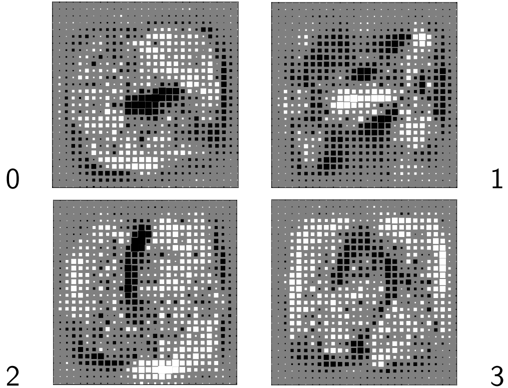


Hinton diagram for single layer network trained on MNIST

- 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)

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)

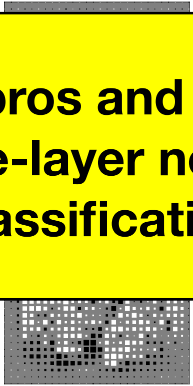


Hinton diagram for single layer network trained on MNIST

- 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)

What are the pros and cons of using a single-layer network for MNIST classification?

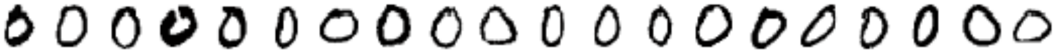
2



3

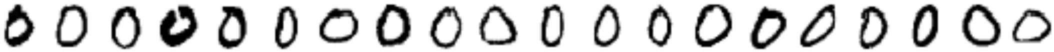
Multi-Layer Networks

From templates to features



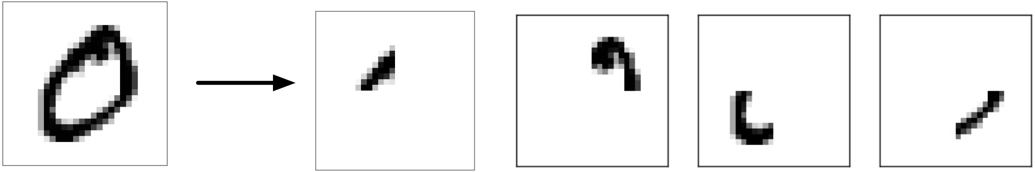
- Good classification needs to cope with the variability of real data: scale, skew, rotation, translation, ...
- Very difficult to do with a single template per class
- Could have multiple templates per task... this will work, but we can do better

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

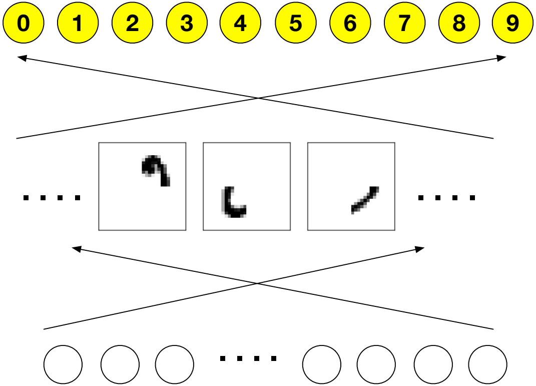
Use features rather than templates



(images from: Nielsen, chapter 1)

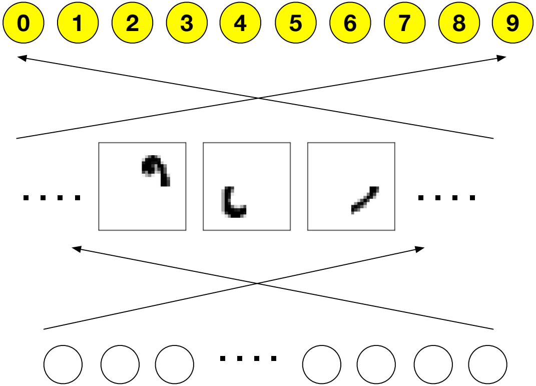
Incorporating features in neural network architecture

Layered processing: inputs - features - classification



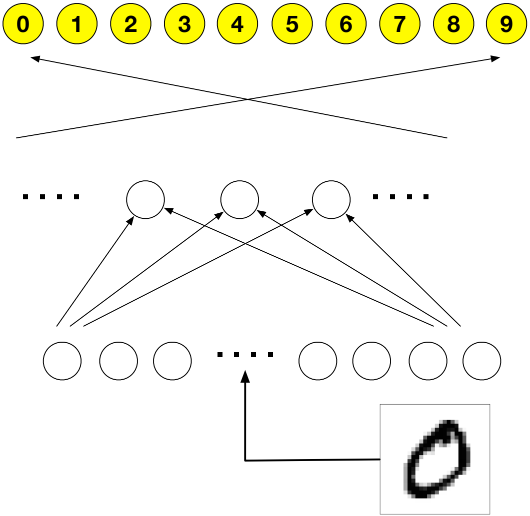
Incorporating features in neural network architecture

Layered processing: inputs - features - classification

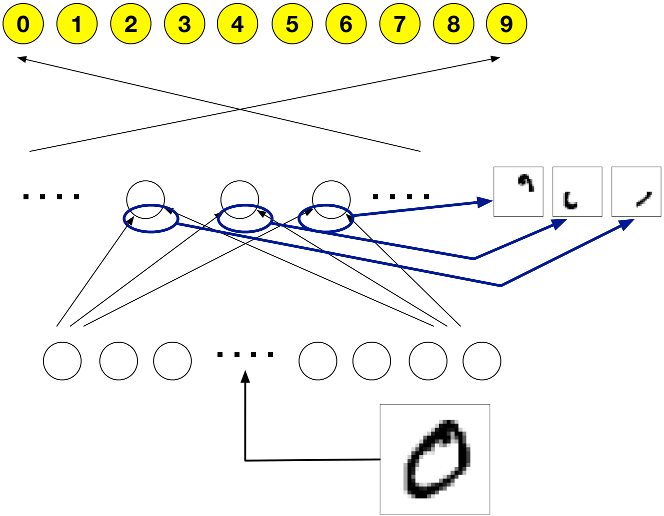


How to obtain features? - learning!

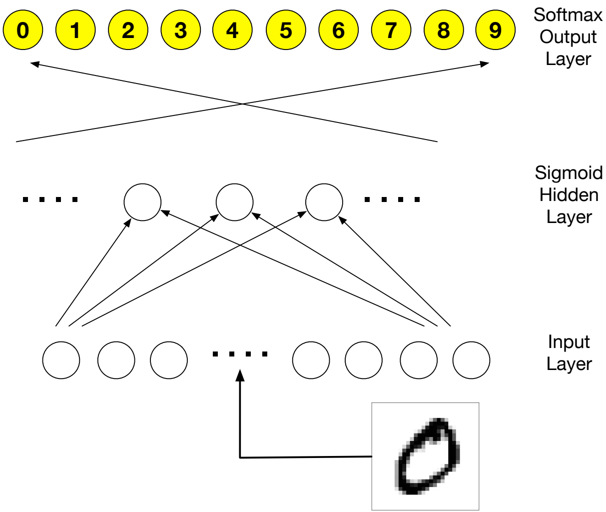
Incorporating features in neural network architecture



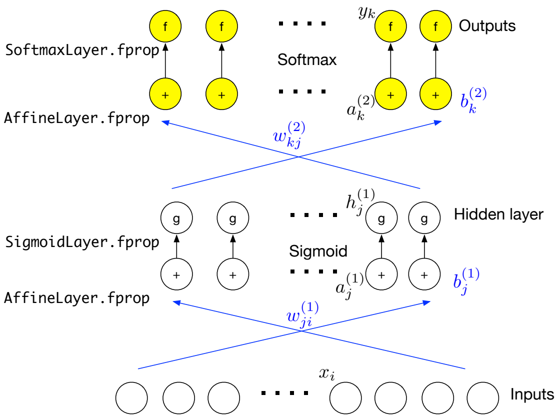
Incorporating features in neural network architecture



Incorporating features in neural network architecture

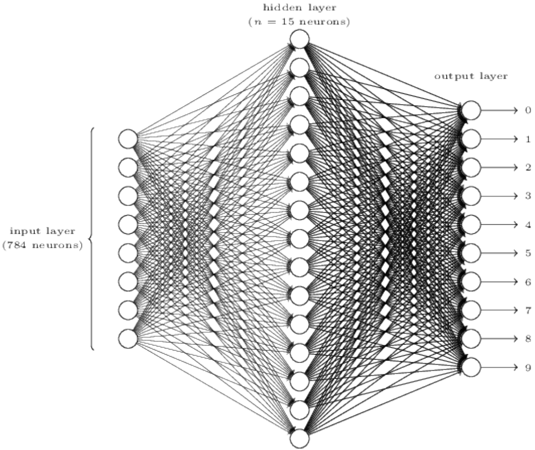


Multi-layer network



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

Multi-layer network for MNIST



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

Training multi-layer networks: 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?

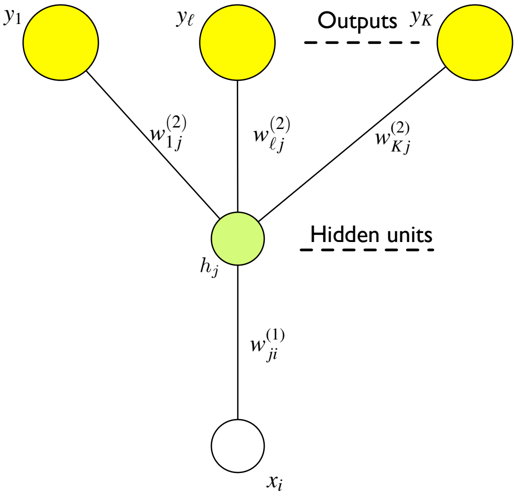
Training multi-layer networks: Credit assignment

- 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?
- *What is the gradient of the error with respect to each weight?*
  (How to compute `grads_wrt_params`?)

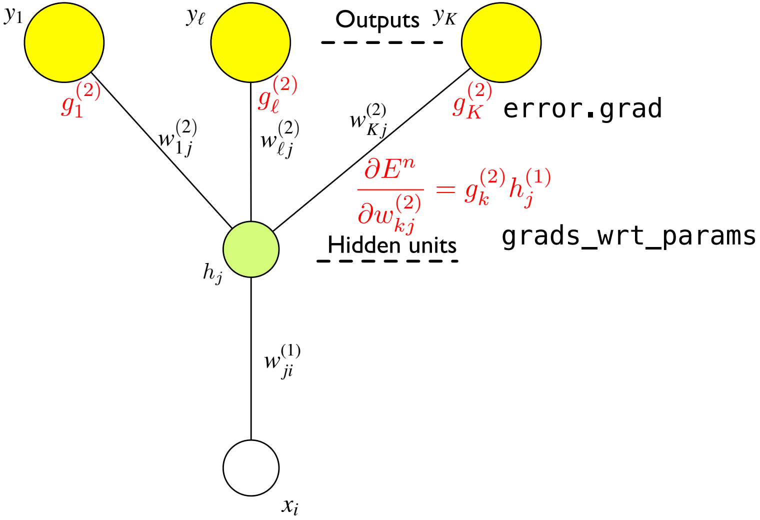
Training multi-layer networks: Credit assignment

- 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?
- *What is the gradient of the error with respect to each weight?* (How to compute `grads_wrt_params`?)
- Solution: *back-propagation of error* (backprop)
- Backprop enables the gradients to be computed. These gradients are used by gradient descent to train the weights.

Training output weights



Training output weights



- Cross-entropy error function:

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

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

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

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

Training MLPs: Error function and required gradients

- Cross-entropy error function:

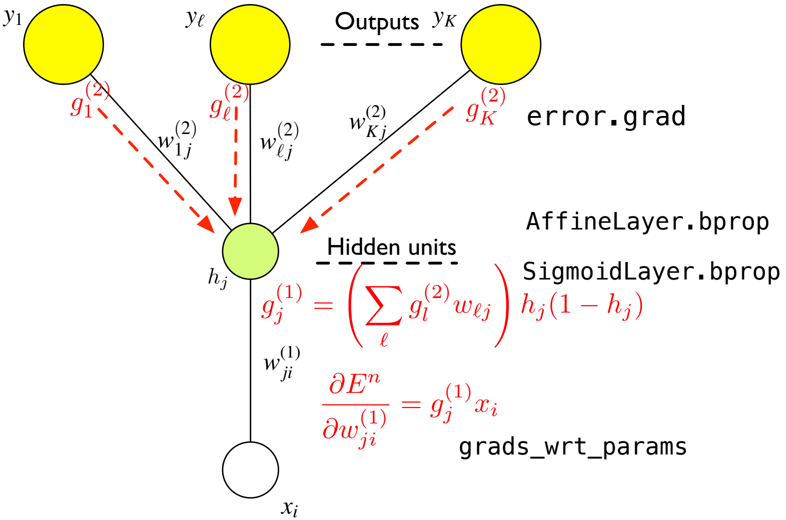
$$E^n = -\sum_{k=1}^{C} t_k^n \ln y_k^n$$

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

$$\underbrace{\boxed{\frac{\partial E^n}{\partial w_{kj}^{(2)}}}}_{\texttt{grads\_wrt\_params}} = \frac{\partial E^n}{\partial z_k^{(2)}} \cdot \frac{\partial z_k^{(2)}}{\partial w_{kj}} = \left(\sum_{c=1}^{C} \frac{\partial E^n}{\partial y_c} \cdot \frac{\partial y_c}{\partial z_k^{(2)}} \right) \cdot \frac{\partial z_k^{(2)}}{\partial w_{kj}}$$

$$= \underbrace{(y_k - t_k)}_{\texttt{error.grad}} h_j^{(1)}$$

Back-propagation of error: hidden unit error signal



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

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

Training MLPs: Input-to-hidden weights

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

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

$$\boxed{g_j^{(1)}} = \sum_{c=1}^{K} \frac{\partial E^n}{\partial z_c^{(2)}} \cdot \frac{\partial z_c^{(2)}}{\partial z_j^{(1)}} = \left(\sum_{c=1}^{K} g_c^{(2)} \cdot \frac{\partial z_c^{(2)}}{\partial h_j^{(1)}} \right) \cdot \frac{\partial h_j^{(1)}}{\partial z_j^{(1)}}$$

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

Training MLPs: Input-to-hidden weights

$$\underbrace{\boxed{\frac{\partial E^n}{\partial w_{ji}^{(1)}}}}_{\texttt{grads\_wrt\_params}} = \underbrace{\boxed{\frac{\partial E^n}{\partial z_j^{(1)}}}}_{g_j^{(1)}} \cdot \underbrace{\frac{\partial z_j^{(1)}}{\partial w_{ji}^{(1)}}}_{x_i}$$

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

$$\boxed{g_j^{(1)}} = \sum_{c=1}^{K} \frac{\partial E^n}{\partial z_c^{(2)}} \cdot \frac{\partial z_c^{(2)}}{\partial z_j^{(1)}} = \left(\sum_{c=1}^{K} g_c^{(2)} \cdot \frac{\partial z_c^{(2)}}{\partial h_j^{(1)}} \right) \cdot \frac{\partial h_j^{(1)}}{\partial z_j^{(1)}}$$

$$= \underbrace{\left(\sum_{c=1}^{K} g_c^{(2)} w_{cj}^{(2)} \right)}_{\texttt{AffineLayer.bprop}} \underbrace{h_j^{(1)}(1 - h_j^{(1)})}_{\texttt{SigmoidLayer.bprop}}$$

Training MLPs: Gradients

- `grads_wrt_params`:

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

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

Training MLPs: Gradients

- `grads_wrt_params`:

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

$$\boxed{\frac{\partial E^n}{\partial w_{ji}^{(1)}}} = \underbrace{\left(\sum_{c=1}^{k} g_c^{(2)} w_{cj}^{(2)}\right)}_{\texttt{AffineLayer.bprop}} \cdot \underbrace{h_j^{(1)}(1 - h_j^{(1)})}_{\texttt{SigmoidLayer.bprop}} \cdot x_i$$

Training MLPs: Gradients

- `grads_wrt_params`:

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

$$\boxed{\frac{\partial E^n}{\partial w_{ji}^{(1)}}} = \underbrace{\left(\sum_{c=1}^{k} g_c^{(2)} w_{cj}^{(2)} \right)}_{\texttt{AffineLayer.bprop}} \cdot \underbrace{h_j^{(1)}(1 - h_j^{(1)})}_{\texttt{SigmoidLayer.bprop}} \cdot x_i$$

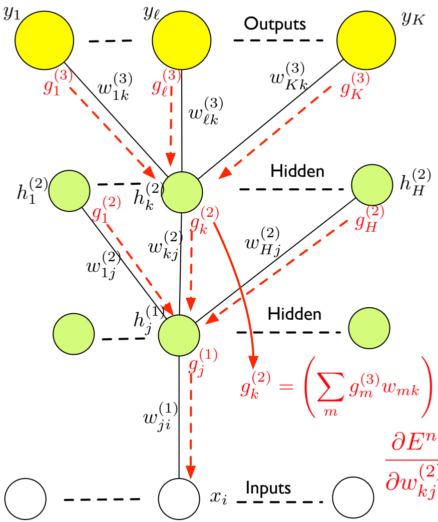
- Exercise: write down expressions for the gradients w.r.t. the biases

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

Back-propagation of error

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

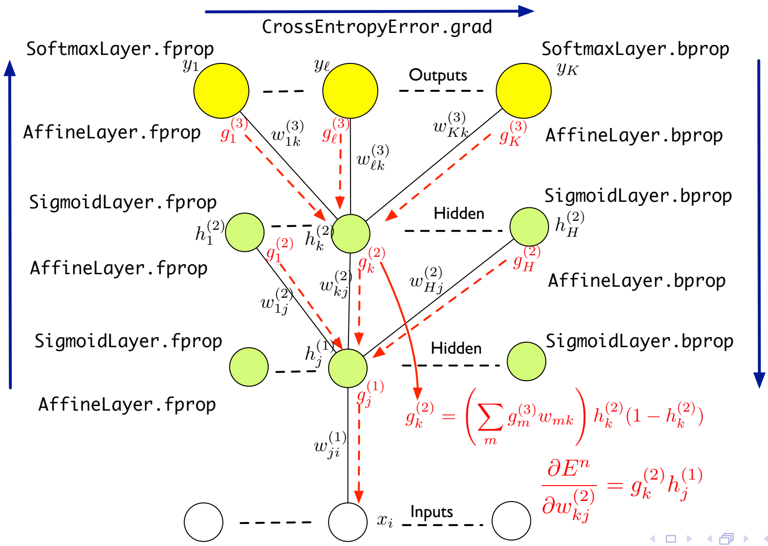
Training with multiple hidden layers



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

$$\frac{\partial E^n}{\partial w_{kj}^{(2)}} = g_k^{(2)} h_j^{(1)}$$

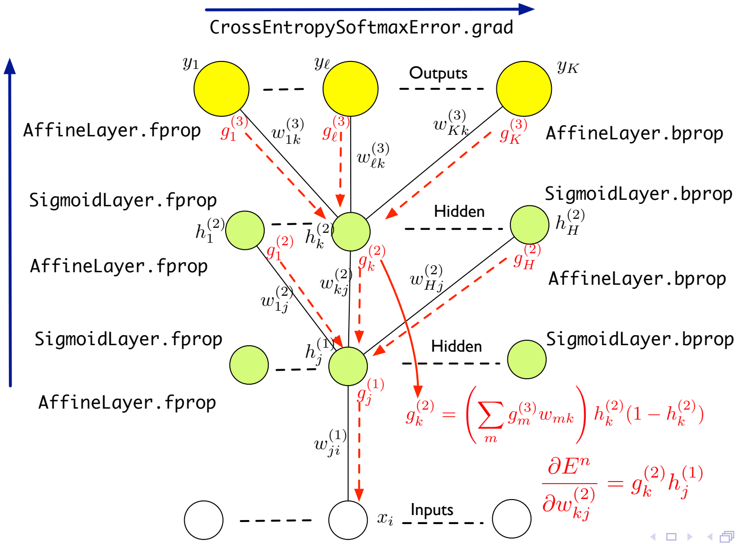
Training with multiple hidden layers



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

$$\frac{\partial E^n}{\partial w_{kj}^{(2)}} = g_k^{(2)} h_j^{(1)}$$

Training with multiple hidden layers

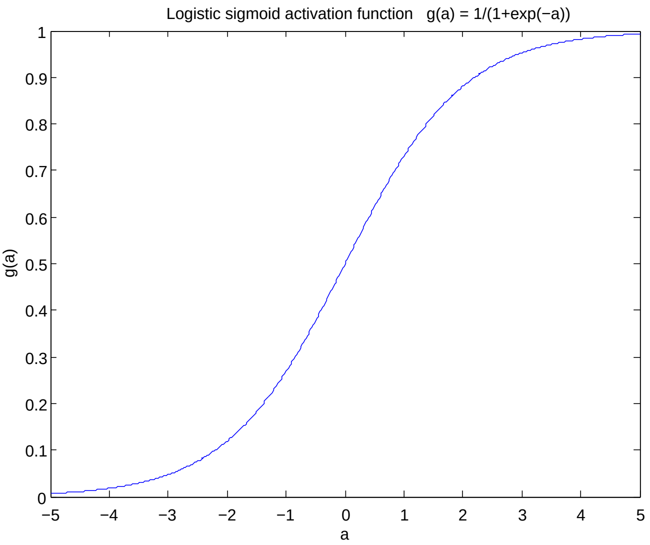


$$g_k^{(2)} = \left(\sum_m g_m^{(3)} w_{mk} \right) h_k^{(2)} (1 - h_k^{(2)})$$

$$\frac{\partial E^n}{\partial w_{kj}^{(2)}} = g_k^{(2)} h_j^{(1)}$$

Are there alternatives to Sigmoid Hidden Units?

Sigmoid function



Sigmoid Hidden Units (`SigmoidLayer`)

- Compress unbounded inputs to (0,1), saturating high magnitudes to 1
- Interpretable as the probability of a feature defined by their weight vector
- Interpretable as the (normalised) firing rate of a neuron

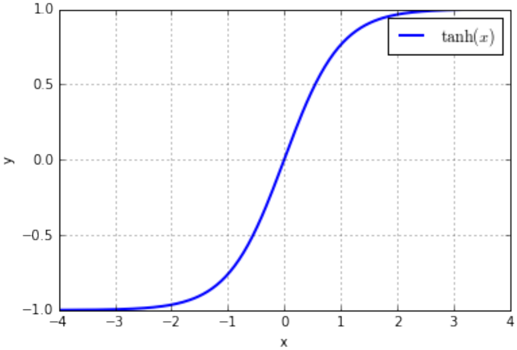
Sigmoid Hidden Units (`SigmoidLayer`)

- Compress unbounded inputs to (0,1), saturating high magnitudes to 1
- Interpretable as the probability of a feature defined by their weight vector
- Interpretable as the (normalised) firing rate of a neuron

However...

- Saturation causes gradients to approach 0
  - If the output of a sigmoid unit is h, then the gradient is $h(1-h)$ which approaches 0 as h saturates to 0 or 1 – hence the gradients it multiplies into approach 0.
  - Small gradients result in small parameter changes, so learning becomes slow
- Outputs are not centred at 0
  - The output of a sigmoid layer will have mean>0 – numerically undesirable.

tanh



$$\tanh(x) = \frac{e^x - e^{-x}}{e^x + e^{-x}}$$

$$\text{sigmoid}(x) = \frac{1 + \tanh(x/2)}{2}$$

Derivative:

$$\frac{d}{dx}\tanh(x) = 1 - \tanh^2(x)$$

tanh hidden units (TanhLayer)

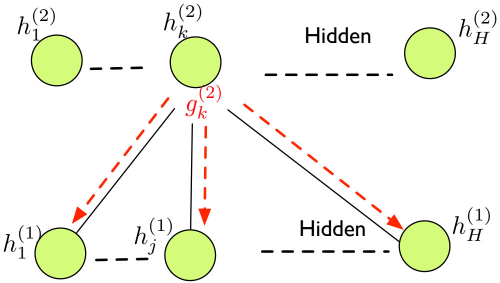
- tanh has same shape as sigmoid but has output range ± 1
- Results about approximation capability using sigmoid layers also apply to tanh layers

tanh hidden units (`TanhLayer`)

- tanh has same shape as sigmoid but has output range ± 1
- Results about approximation capability using sigmoid layers also apply to tanh layers
- Possible reason to prefer tanh over sigmoid: allowing units to be positive or negative allows gradient for weights into a hidden unit to have a different sign

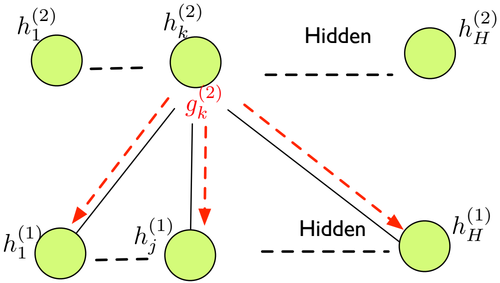
tanh hidden units (TanhLayer)

- tanh has same shape as sigmoid but has output range ± 1
- Results about approximation capability using sigmoid layers also apply to tanh layers
- Possible reason to prefer tanh over sigmoid: allowing units to be positive or negative allows gradient for weights into a hidden unit to have a different sign

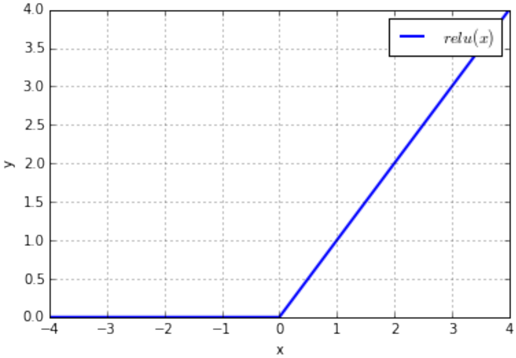


tanh hidden units (TanhLayer)

- tanh has same shape as sigmoid but has output range ± 1
- Results about approximation capability using sigmoid layers also apply to tanh layers
- Possible reason to prefer tanh over sigmoid: allowing units to be positive or negative allows gradient for weights into a hidden unit to have a different sign
- Saturation still a problem



Rectified Linear Unit – ReLU



$$\text{relu}(x) = \max(0, x)$$

Derivative:

$$\frac{d}{dx}\text{relu}(x) = \begin{cases} 0 & \text{if } x \leq 0 \\ 1 & \text{if } x > 0 \end{cases}$$

ReLU hidden units (`ReluLayer`)

- Similar approximation results to tanh and sigmoid hidden units
- Empirical results for speech and vision show consistent improvements using relu over sigmoid or tanh
- Unlike tanh or sigmoid there is no positive saturation – saturation results in very small derivatives (and hence slower learning)

ReLU hidden units (`ReluLayer`)

- Similar approximation results to tanh and sigmoid hidden units
- Empirical results for speech and vision show consistent improvements using relu over sigmoid or tanh
- Unlike tanh or sigmoid there is no positive saturation – saturation results in very small derivatives (and hence slower learning)

- Negative input to relu results in zero gradient (and hence no learning)
- Relu is computationally efficient: $\max(0, x)$
- Relu units can "die" (i.e. respond with 0 to everything)
- Relu units can be very sensitive to the learning rate

Lab 3: 03_Multiple_layer_models

Lab 3 covers how multiple layer networks are modelled in the `mlp` framework.

- Representing activation functions as layer, applied after a linear (affine) layer
- Stacking layers together to build multi-layer networks with non-linear activation functions (e.g. sigmoid) for the hidden layer
- Using `Layer.fprop` methods to implement the forward propagation and and `Layer.bprop` methods to implement back propagation to compute the gradients
- Training softmax models on MNIST
- Training deeper multi-layer networks on MNIST
- Using various non-linear activation functions for the hidden layer (sigmoid, tanh, relu)

Summary

- Understanding what single-layer networks compute
- How multi-layer networks allow feature computation
- Training multi-layer networks using back-propagation of error
- Tanh and ReLU activation functions
- Multi-layer networks are also referred to as *deep neural networks* or *multi-layer perceptrons*
- **Reading**:
  - Nielsen, chapter 2
  - Goodfellow, sections 6.3, 6.4, 6.5
  - Bishop, sections 3.1, 3.2, and chapter 4