Machine Learning – COMS3007

Neural Networks

(Learning)

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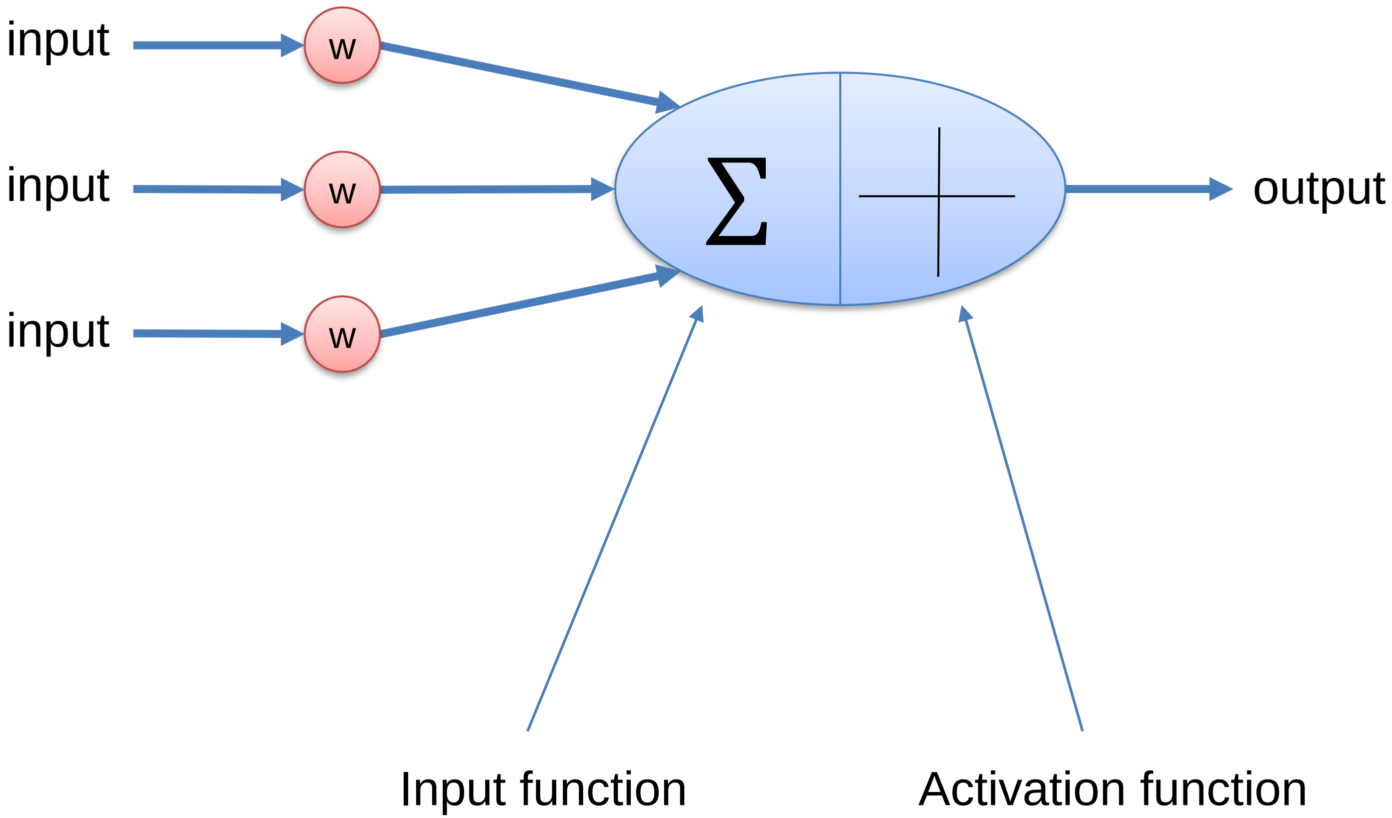
Based heavily on course notes by Geoffrey Hinton, Chris Williams and Victor Lavrenko, Amos Storkey, Eric Eaton, and Clint van Alten

Neuron anatomy

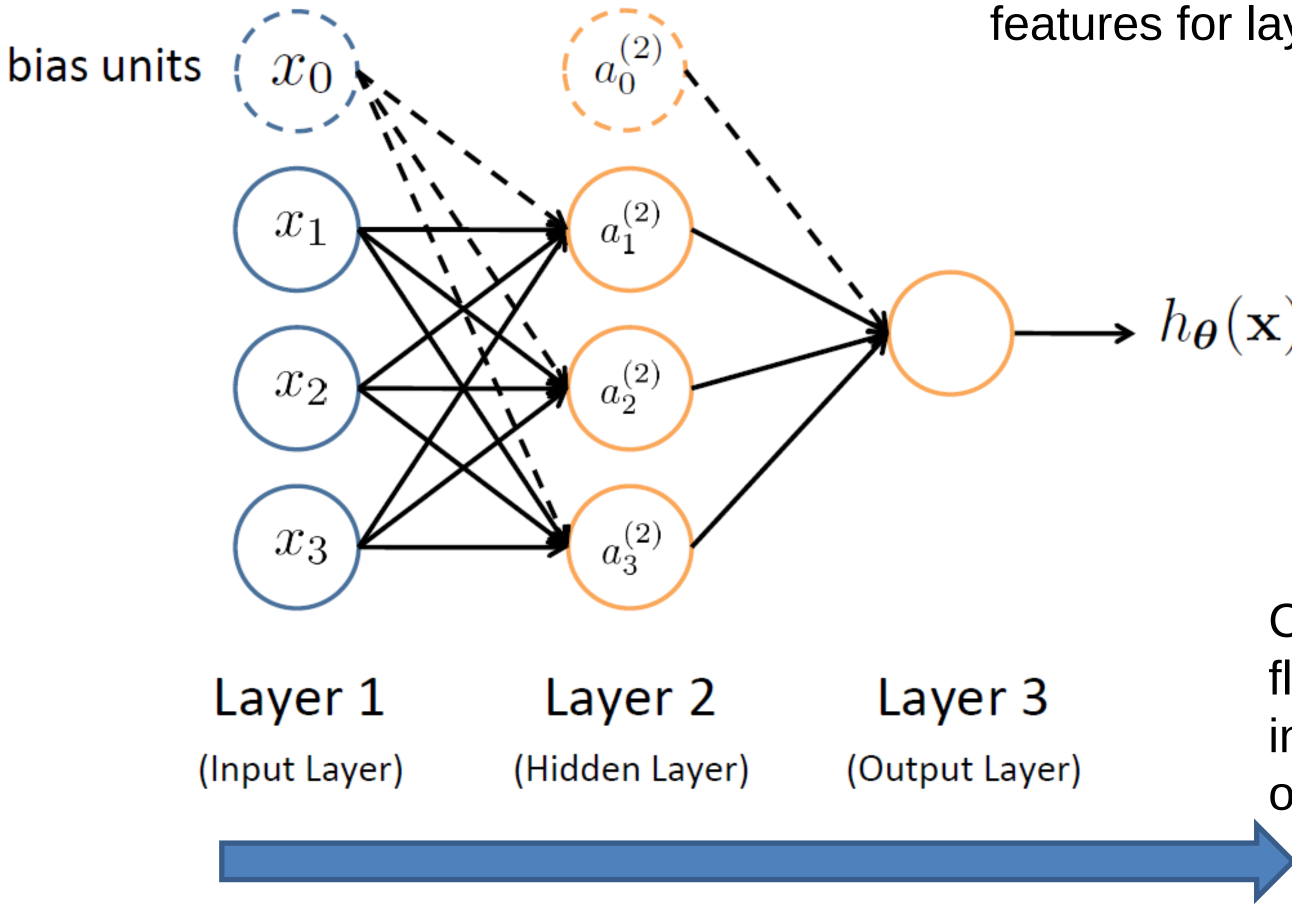


- Intuition: stack these neurons to learn features!

Stacking neurons

- Neurons arranged in layers

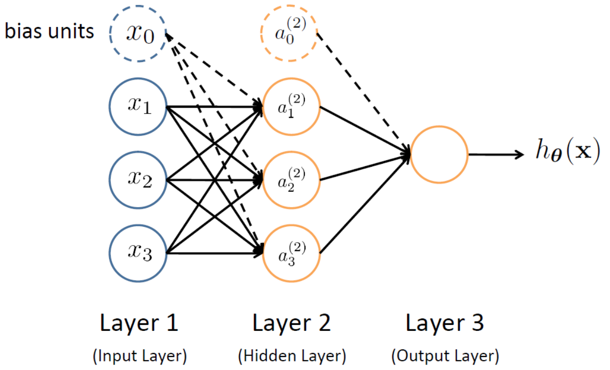
Layer n acts as features for layer n+1



Computation flows from input to output

Feed-forward networks

Sometimes called multilayer perceptrons (MLPs)



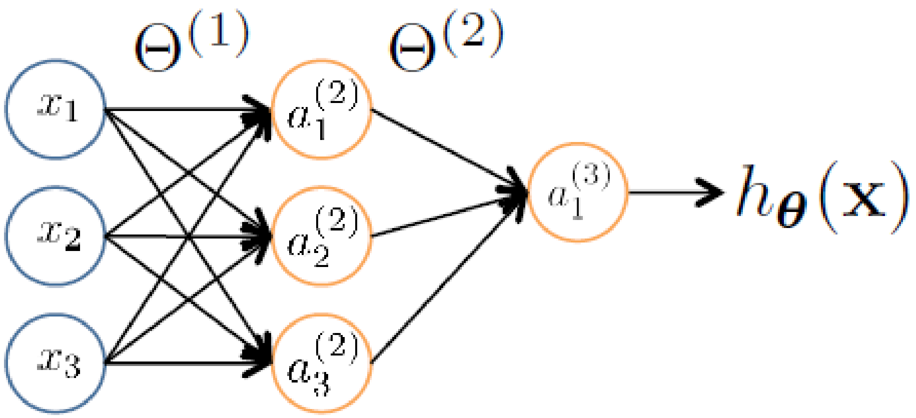
- Input layers
  - Raw data
  - As provided by sensor measurements

- Feed-forward networks (most common)
  - Outputs from one layer become inputs to the next

- Working forward through the network:
  - Apply input function to compute total input
    - Usually just the sum of inputs
  - Activation function transforms input to final value
    - Usually nonlinear function

- Output layer: computation target

Vectorization



- $a_1^{(2)} = g\left(\Theta_{10}^{(1)} x_0 + \Theta_{11}^{(1)} x_1 + \Theta_{12}^{(1)} x_2 + \Theta_{13}^{(1)} x_3\right) = g(z_1^{(2)})$
- $a_2^{(2)} = g\left(\Theta_{20}^{(1)} x_0 + \Theta_{21}^{(1)} x_1 + \Theta_{22}^{(1)} x_2 + \Theta_{23}^{(1)} x_3\right) = g(z_2^{(2)})$
- $a_3^{(2)} = g\left(\Theta_{30}^{(1)} x_0 + \Theta_{31}^{(1)} x_1 + \Theta_{32}^{(1)} x_2 + \Theta_{33}^{(1)} x_3\right) = g(z_3^{(2)})$
- $h_\Theta(x) = g\left(\Theta_{10}^{(2)} a_0^{(2)} + \Theta_{11}^{(2)} a_1^{(2)} + \Theta_{12}^{(2)} a_2^{(2)} + \Theta_{13}^{(2)} a_3^{(2)}\right) = g(z_1^{(3)})$

Vectorized steps:

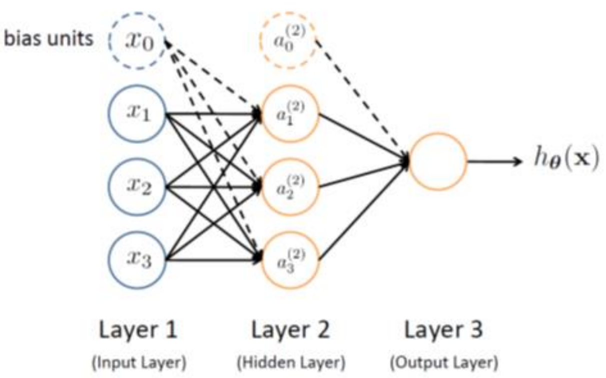
- $\boldsymbol{z}^{(2)} = \Theta^{(1)} \boldsymbol{x}$
- $\boldsymbol{a}^{(2)} = g(\boldsymbol{z}^{(2)})$
- Add $a_0^{(2)} = 1$
- $\boldsymbol{z}^{(3)} = \Theta^{(2)} \boldsymbol{a}^{(2)}$
- $h_\Theta(\boldsymbol{x}) = \boldsymbol{a}^{(3)} = g(\boldsymbol{z}^{(3)})$

Perceptron Learning Rule

Target (y)	Predicted (h(x))	Bracket (y-h(x))	Update
0	0	0	0
0	1	-1	$-\alpha x$
1	0	1	αx
1	1	0	0

- $\theta \leftarrow \theta + \alpha\big(y - h(x)\big)x$
- Intuition:
  - If output is correct ($y = h(x)$):
    - Don't change weights
  - If output too low ($h(x) = 0, y = 1$):
    - Increment weights
  - If output too high ($h(x) = 1, y = 0$):
    - Decrement weights
- If the data is linearly separable (set of consistent weights exists): guaranteed to converge.

Learning in a NN



- Similar to perceptron learning:
  - Cycle through training examples
  - If network output is correct, no changes are made
  - If there is an error, adjust weights to reduce error
- We are just performing (stochastic) gradient descent
- Challenge:
  - It’s easy to talk about error in the output layer, but what about the hidden layers?
    - We need to assign “blame” to the weights that need to change

Cost functions

n = number of datapoints
K = number of output classes
L = number of layers
s_l = number of neurons on layer l
Θ = weight matrix

- Logistic regression:
- $J(\boldsymbol{\theta}) = -\frac{1}{n}\sum_{i=1}^{n}\left[y_i \log h_{\boldsymbol{\theta}}(\boldsymbol{x}_i) + (1-y_i)\log\left(1-h_{\boldsymbol{\theta}}(\boldsymbol{x}_i)\right)\right] + \frac{\lambda}{2n}\sum_{j=1}^{d}\theta_j^2$
- Neural network:
- $h_\Theta \in \mathbb{R}^K$
- $(h_\Theta(\boldsymbol{x}))_i$ = i^th^ output
- $J(\Theta) = -\frac{1}{n}\left[\sum_{i=1}^{n}\sum_{k=1}^{K} y_{ik}\log\left(h_\Theta(\boldsymbol{x}_i)\right)_k + (1-y_{ik})\log\left(1-\left(h_\Theta(\boldsymbol{x}_i)\right)_k\right)\right] + \frac{\lambda}{2n}\sum_{l=1}^{L-1}\sum_{i=1}^{s_{l-1}}\sum_{j=1}^{s_l}\left(\Theta_{ji}^{(l)}\right)^2$
- This is for classification. The error changes if the task changes.
- E.g. regression: $J(\Theta) = \frac{1}{2n}\sum_{i=1}^{n}(h_\Theta(\boldsymbol{x}_i) - y_i)^2$

Optimising the NN

$$J(\Theta) = -\frac{1}{n}\left[\sum_{i=1}^{n}\sum_{k=1}^{K} y_{ik}\log\left(h_\Theta(\boldsymbol{x}_i)\right)_k + (1-y_{ik})\log\left(1-\left(h_\Theta(\boldsymbol{x}_i)\right)_k\right)\right] + \frac{\lambda}{2n}\sum_{l=1}^{L-1}\sum_{i=1}^{s_{l-1}}\sum_{j=1}^{s_l}\left(\Theta_{ji}^{(l)}\right)^2$$

- Solve as $\min_{\Theta} J(\Theta)$
  - No closed-form solution in general
    - Use iterative solution (GD)
  - Also: this is not convex, so GD on a neural net will give us a local optimum

- Gradient descent:
  - For each parameter $\Theta_{ji}^{(l)}$:
    - $\Theta_{ji}^{(l)} \leftarrow \Theta_{ji}^{(l)} - \alpha \dfrac{\partial J(\Theta)}{\partial \Theta_{ji}^{(l)}}$

Learning rate

Optimising the NN

- So, need to be able to compute:
  - $\frac{\partial}{\partial \Theta_{ij}^{(l)}} J(\Theta)$ - the gradient of the error wrt all the parameters
    - Use the chain rule to compute: called backpropagation in ANNs
    - Compute backwards by layer from output layer to input layer

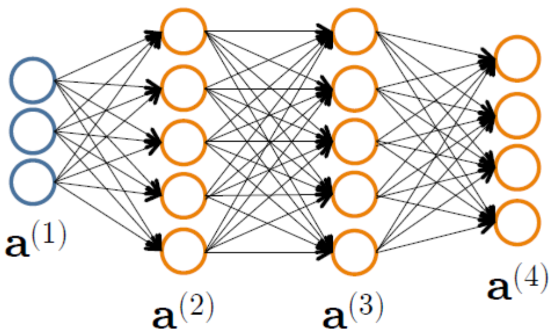
    - How to compute this?
      - $\frac{\partial}{\partial \Theta_{ij}^{(l)}} J(\Theta)$ = (influence of connection) x (error at next layer)

      - $= a_j^{(l)} \delta_i^{(l+1)}$ (ignoring regularization)

Forward propagation backpropagation

Forward propagation

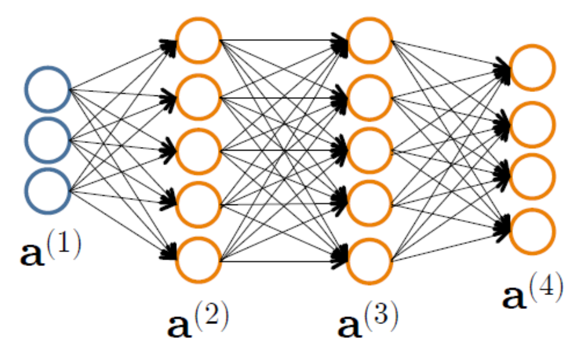
- Given one labelled training instance $(\boldsymbol{x}, y)$:
- Compute activations $\boldsymbol{y}^{(i)}$



- Forward propagation:
  - $\boldsymbol{a}^{(1)} = \boldsymbol{x}$
  - $\boldsymbol{z}^{(2)} = \Theta^{(1)}\boldsymbol{a}^{(1)}$
  - $\boldsymbol{a}^{(2)} = g(\boldsymbol{z}^{(2)})$ [add $a_0^{(2)}$]
  - $\boldsymbol{z}^{(3)} = \Theta^{(2)}\boldsymbol{a}^{(2)}$
  - $\boldsymbol{a}^{(3)} = g(\boldsymbol{z}^{(3)})$ [add $a_0^{(3)}$]
  - $\boldsymbol{z}^{(4)} = \Theta^{(3)}\boldsymbol{a}^{(3)}$
  - $\boldsymbol{a}^{(4)} = h_\Theta(\boldsymbol{x}) = g(\boldsymbol{z}^{(4)})$

Backpropagation intuition

- Forward prop gave us the activations $\boldsymbol{a}$
- Each hidden node j is “responsible” for some fraction of the **error $\boldsymbol{\delta_j^{(l)}}$ in each of the output nodes** to which it connects
- $\delta_j^{(l)}$ is divided according to the **strength of the connection** between hidden node and output node
- Then, the “blame” is propagated back to provide error values for the hidden layer



Backpropagation derivation

- We need to be able to compute the derivative: $\dfrac{\partial J(\Theta)}{\partial \Theta_{ij}^{(l-1)}}$

- $\dfrac{\partial J}{\partial \theta_{ij}^{(l-1)}} = \dfrac{\partial J}{\partial a_i^{(l)}} \dfrac{\partial a_i^{(l)}}{\partial z_i^{(l)}} \dfrac{\partial z_i^{(l)}}{\partial \theta_{ij}^{(l-1)}}$ (chain rule)

$$\boldsymbol{a}^{(l)} = g\left(\boldsymbol{z}^{(l)}\right)$$

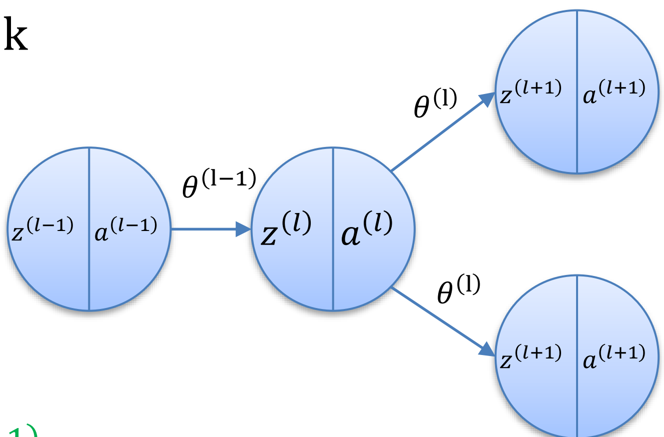
$$\boldsymbol{z}^{(l)} = \Theta^{(l-1)} \boldsymbol{a}^{(l-1)}$$

- $\dfrac{\partial J}{\partial a_i^{(l)}} = \sum_m \dfrac{\partial J}{\partial z_m^{(l+1)}} \dfrac{\partial z_m^{(l+1)}}{\partial a_i^{(l)}} = \sum_m \dfrac{\partial J}{\partial z_m^{(l+1)}} \theta_{mi}^{(l)}$ (sum over next neurons)

- Let $\delta_k^{(l)} = \dfrac{\partial J}{\partial z_k^{(l)}}$ be the change in error from node k

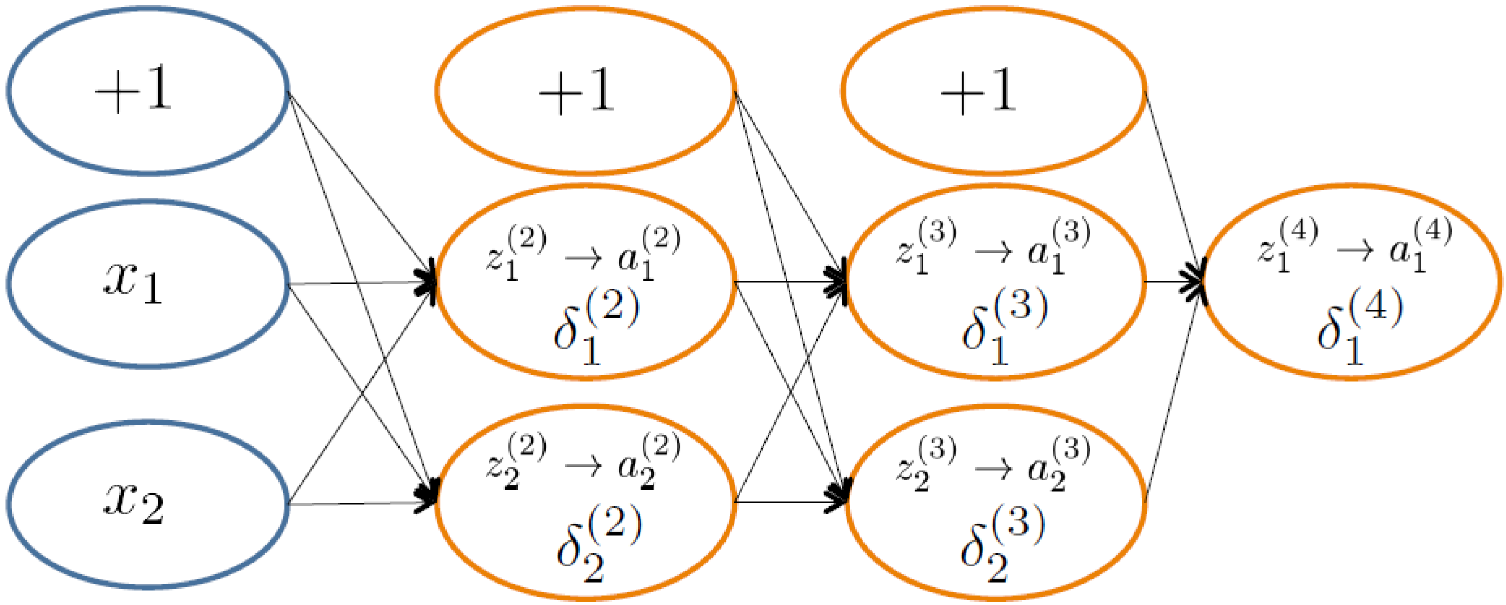
- $\dfrac{\partial a_i^{(l)}}{\partial z_i^{(l)}} = g'\left(z_i^{(l)}\right)$

- $\dfrac{\partial z_i^{(l)}}{\partial \theta_{ij}^{(l-1)}} = a_j^{(l-1)}$



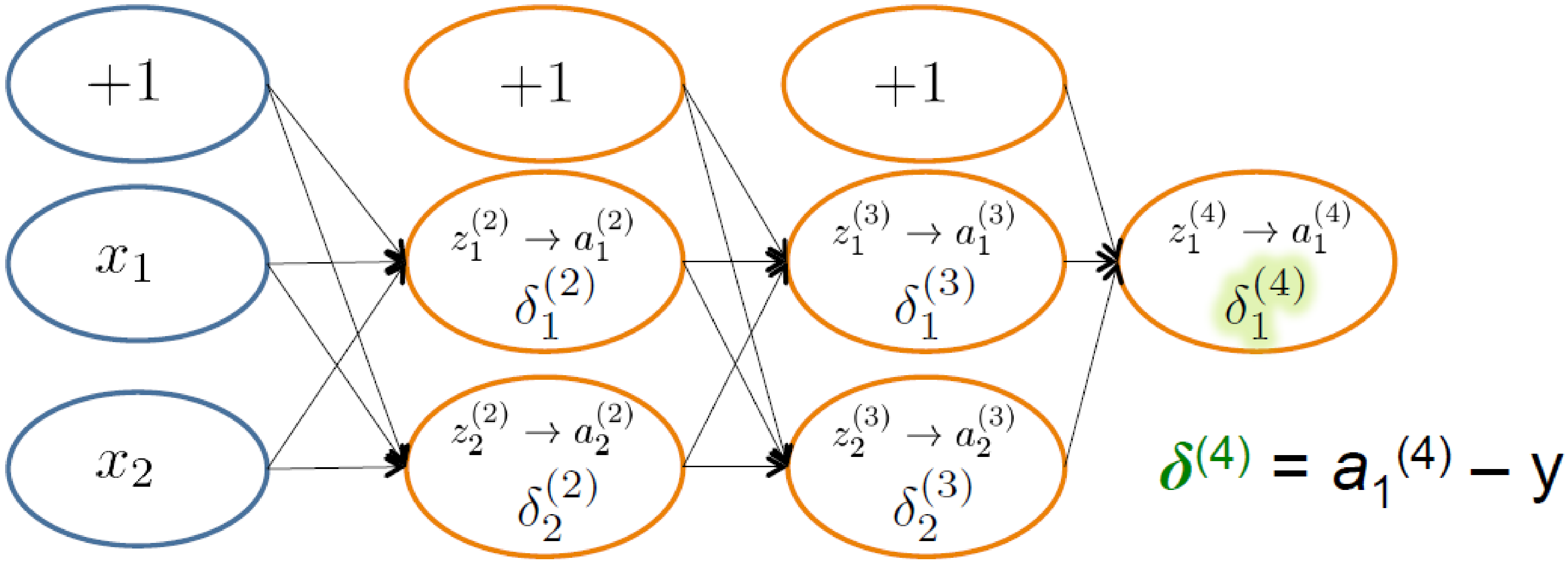
- Therefore: $\dfrac{\partial J}{\partial \theta_{ij}^{(l-1)}} = \overbrace{\left(\sum_m \delta_m^{(l+1)} \theta_{mi}^{(l)}\right) g'\left(z_i^{(l)}\right)}^{\delta_i^{(l)}} a_j^{(l-1)}$

Backpropagation intuition



- $\delta_j^{(l)}$ = "error" of node j in layer l
- Formally, $\delta_j^{(l)} = \frac{\partial}{\partial z_j^{(l)}} J(\boldsymbol{x}_i)$

Backpropagation intuition



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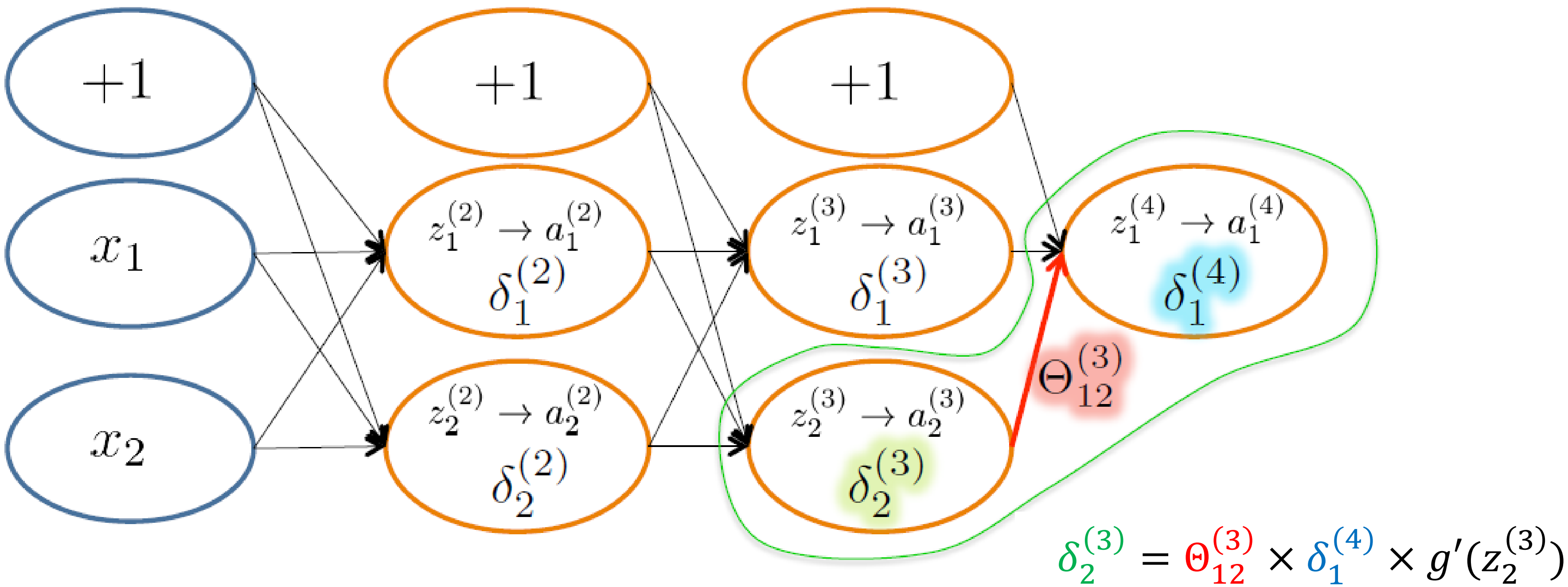

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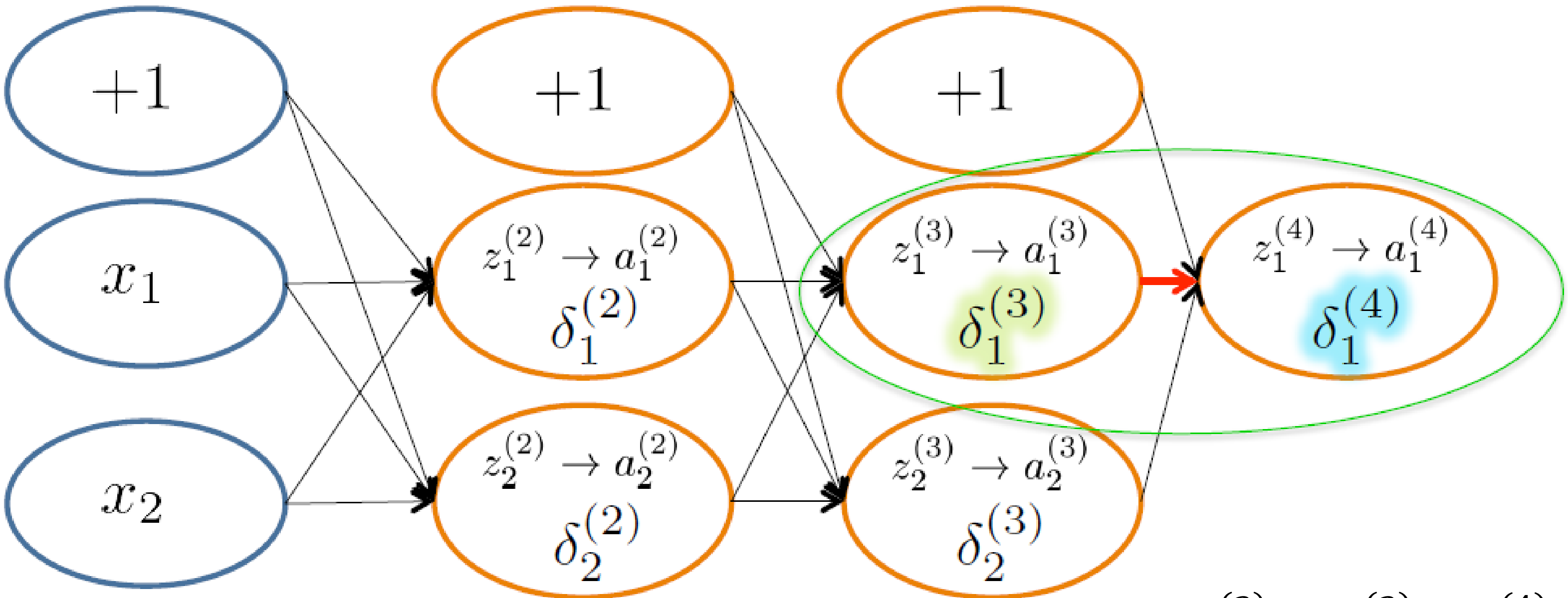
Backpropagation intuition



$$\delta_2^{(3)} = \Theta_{12}^{(3)} \times \delta_1^{(4)} \times g'(z_2^{(3)})$$

$$\delta_1^{(3)} = \Theta_{11}^{(3)} \times \delta_1^{(4)} \times g'(z_1^{(3)})$$

- $\delta_j^{(l)}$ = "error" of node j in layer l
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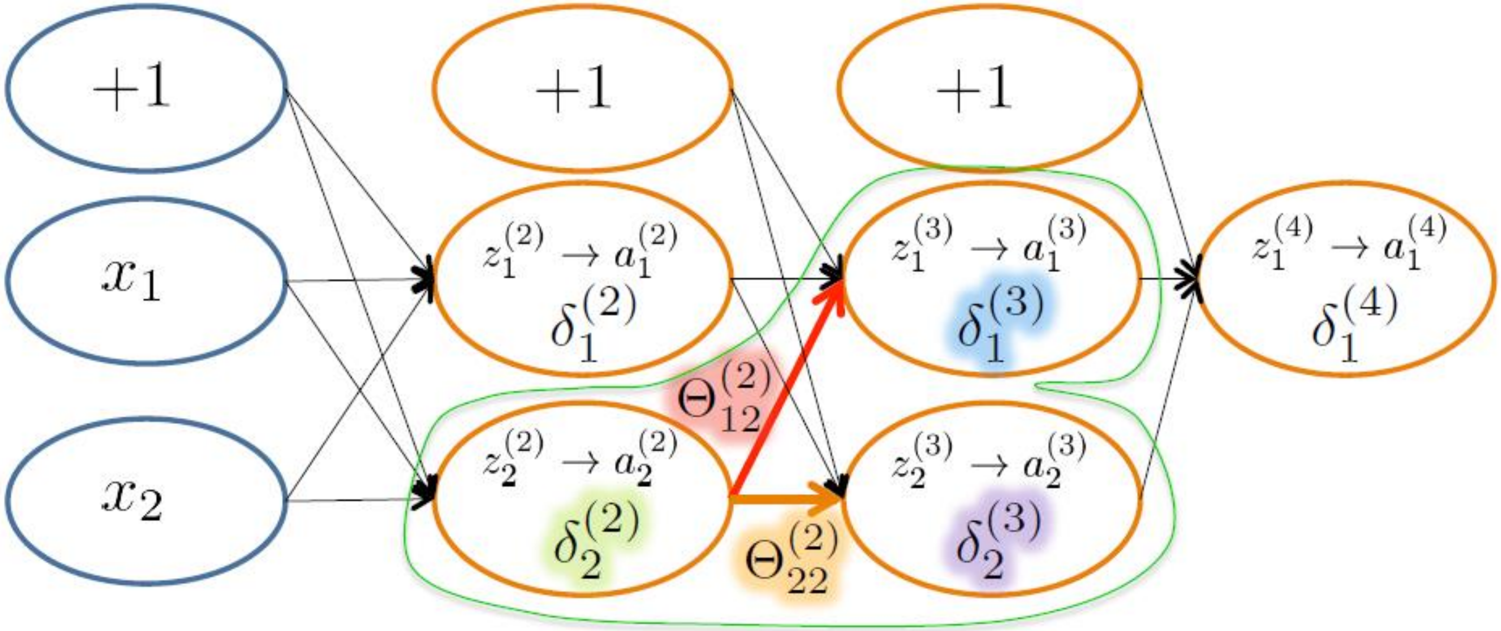
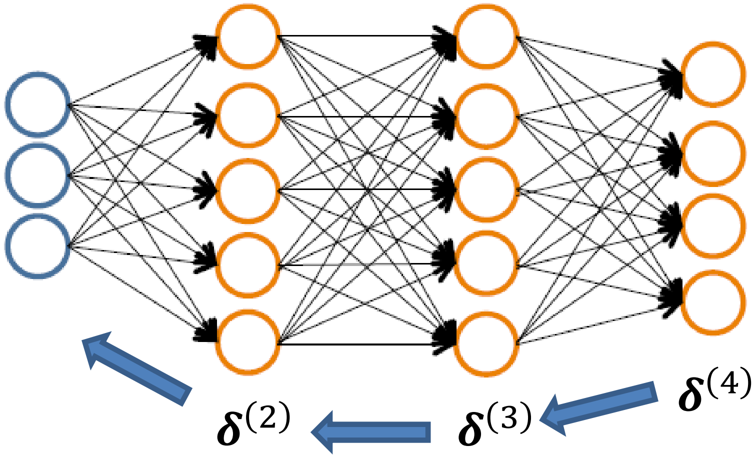
Backpropagation intuition



$$\delta_2^{(2)} = \Theta_{12}^{(2)} \times \delta_1^{(3)} \times g'(z_2^{(2)}) + \Theta_{22}^{(2)} \times \delta_2^{(3)} \times g'(z_2^{(2)})$$

- $\delta_j^{(l)}$ = "error" of node j in layer l
- Formally, $\delta_j^{(l)} = \frac{\partial}{\partial z_j^{(l)}} J(\boldsymbol{x}_i)$

Backpropagation intuition



- $\delta_j^{(l)}$ = "error" of node j in layer l

- Backprop:
- $\boldsymbol{\delta}^{(4)} = \boldsymbol{a}^{(4)} - \boldsymbol{y}$
- $\boldsymbol{\delta}^{(3)} = \left(\Theta^{(3)}\right)^T \boldsymbol{\delta}^{(4)} \times g'\left(\boldsymbol{z}^{(3)}\right)$
- $\boldsymbol{\delta}^{(2)} = \left(\Theta^{(2)}\right)^T \boldsymbol{\delta}^{(3)} \times g'\left(\boldsymbol{z}^{(2)}\right)$
- No $\boldsymbol{\delta}^{(1)}$ - no error in inputs

If g is a sigmoid:

$g'\left(\boldsymbol{z}^{(3)}\right) = \boldsymbol{a}^{(3)}\left(1 - \boldsymbol{a}^{(3)}\right)$

$g'\left(\boldsymbol{z}^{(2)}\right) = \boldsymbol{a}^{(2)}\left(1 - \boldsymbol{a}^{(2)}\right)$

- $\frac{\partial}{\partial \Theta_{ij}^{(l)}} J(\Theta) = a_j^{(l)} \delta_i^{(l+1)}$

Backpropagation algorithm

Set $\Delta_{ij}^{(l)} = 0, \ \forall l, i, j$

For each training instance $(\boldsymbol{x}_i, y_i)$:

Set $\boldsymbol{a}^{(1)} = \boldsymbol{x}_i$

Compute $\{\boldsymbol{a}^{(2)}, \dots, \boldsymbol{a}^{(L)}\}$ with forward propagation

Compute $\boldsymbol{\delta}^{(L)} = \boldsymbol{a}^{(L)} - y_i$

Compute errors $\{\boldsymbol{\delta}^{(L-1)}, \dots, \boldsymbol{\delta}^{(2)}\}$

Compute gradients $\Delta_{ij}^{(l)} = \Delta_{ij}^{(l)} + a_j^{(l)} \delta_i^{(l+1)}$

Don't regularise the bias

Compute average regularised gradient $D_{ij}^{(l)} = \begin{cases} \frac{1}{n}\Delta_{ij}^{(l)} + \lambda\Theta_{ij}^{(l)} & if\ j \neq 0 \\ \frac{1}{n}\Delta_{ij}^{(l)} & otherwise \end{cases}$

- $\boldsymbol{D}^{(l)}$ is the matrix of partial derivatives of $J(\Theta)$
- Note: can vectorise $\Delta_{ij}^{(l)} = \Delta_{ij}^{(l)} + a_j^{(l)} \delta_i^{(l+1)}$ as $\boldsymbol{\Delta}^{(\mathrm{l})} = \boldsymbol{\Delta}^{(l)} + \boldsymbol{\delta}^{(l+1)} {\boldsymbol{a}^{(l)}}^T$

Training a NN with GD and Backprop

Given: training data $\{(\boldsymbol{x}_1, y_1), \dots, (\boldsymbol{x}_n, y_n)\}$
Initialise all $\Theta^{(l)}$ randomly (NOT to 0)
Loop (for each epoch):

Set $\Delta_{ij}^{(l)} = 0, \ \ \forall l, i, j$
For each training instance $(\boldsymbol{x}_i, y_i)$:

Set $\boldsymbol{a}^{(1)} = \boldsymbol{x}_i$
Compute $\{\boldsymbol{a}^{(2)}, \dots, \boldsymbol{a}^{(L)}\}$ with forward propagation
Compute $\boldsymbol{\delta}^{(L)} = \boldsymbol{a}^{(L)} - y_i$
Compute errors $\{\boldsymbol{\delta}^{(L-1)}, \dots, \boldsymbol{\delta}^{(2)}\}$
Compute gradients $\Delta_{ij}^{(l)} = \Delta_{ij}^{(l)} + a_j^{(l)} \delta_i^{(l+1)}$

Compute average regularised gradient $D_{ij}^{(l)} = \begin{cases} \frac{1}{n}\Delta_{ij}^{(l)} + \lambda\Theta_{ij}^{(l)} & if\ j \neq 0 \\ \frac{1}{n}\Delta_{ij}^{(l)} & otherwise \end{cases}$

Backpropagation

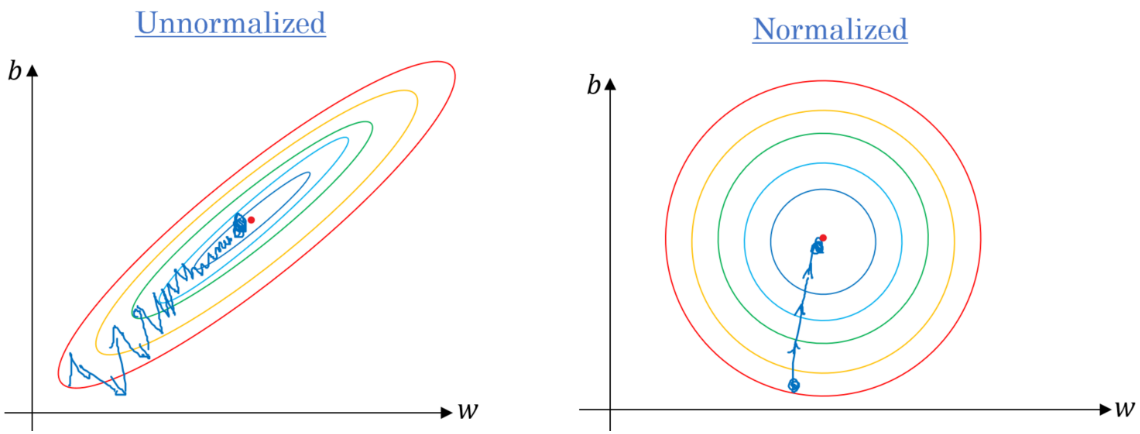
Update weights via gradient step $\Theta_{ij}^{(l)} = \Theta_{ij}^{(l)} - \alpha D_{ij}^{(l)}$
Until weights converge or max epochs reached

Implementation: initialisation

- If two hidden units have:
  - The same bias
  - The same incoming and outgoing weights
- Then they will always get the exact same gradient!
  - Can never learn to be different features
  - Break symmetry by initialising weights to small random values
    - And specifically Gaussian random numbers

Implementation: normalisation

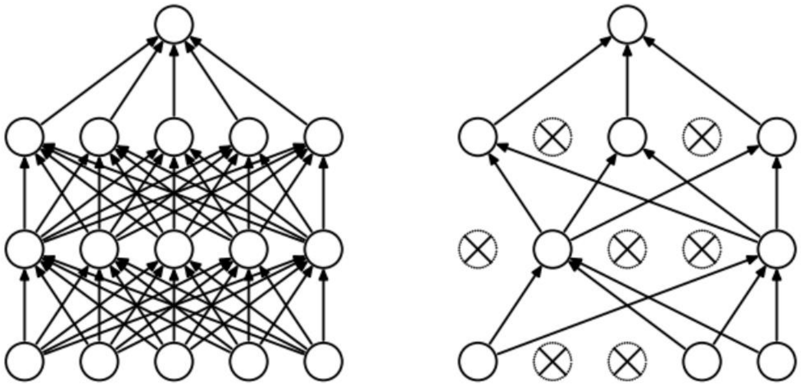
- When training data features have different scales, learning can be slower



- Scale (normalise) features to lie in the same intervals
  - Either: set means to 0, variances to 1 $x \leftarrow \dfrac{x - mean(x)}{variance(x)}$
  - Or: min to 0, max to 1 $x \leftarrow \dfrac{x - min(x)}{max(x) - \min(x)}$

Implementation: dropout

- Neural networks often have a large number of parameters
  - Leads to overfitting

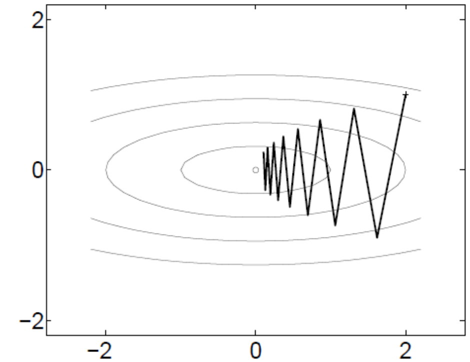


(a) Standard Neural Net (b) After applying dropout.

- Dropout:
  - While training, at each stage, with probability p remove a node and all its connections
    - Another hyperparameter!
    - Prevents network from becoming too dependent on any one node
  - While testing, use all nodes

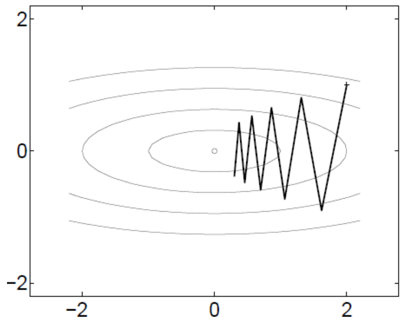
Implementation: momentum

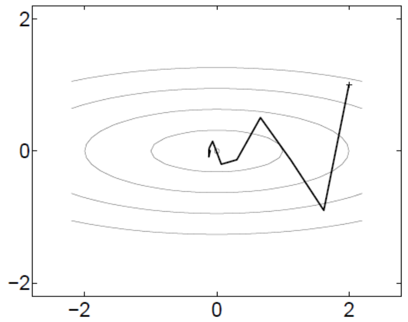
- GD often ends up “zig-zagging” in ravines
- Use momentum:
  - “slow changes in direction”
  - A ball rolling down a hill
  - Another hyperparameter



- Let change in weight θ at time t be $\delta\theta(t)$
- Then $\delta\theta(t+1) = -\alpha\frac{\partial J}{\partial\theta} + \beta\delta\theta(t)$

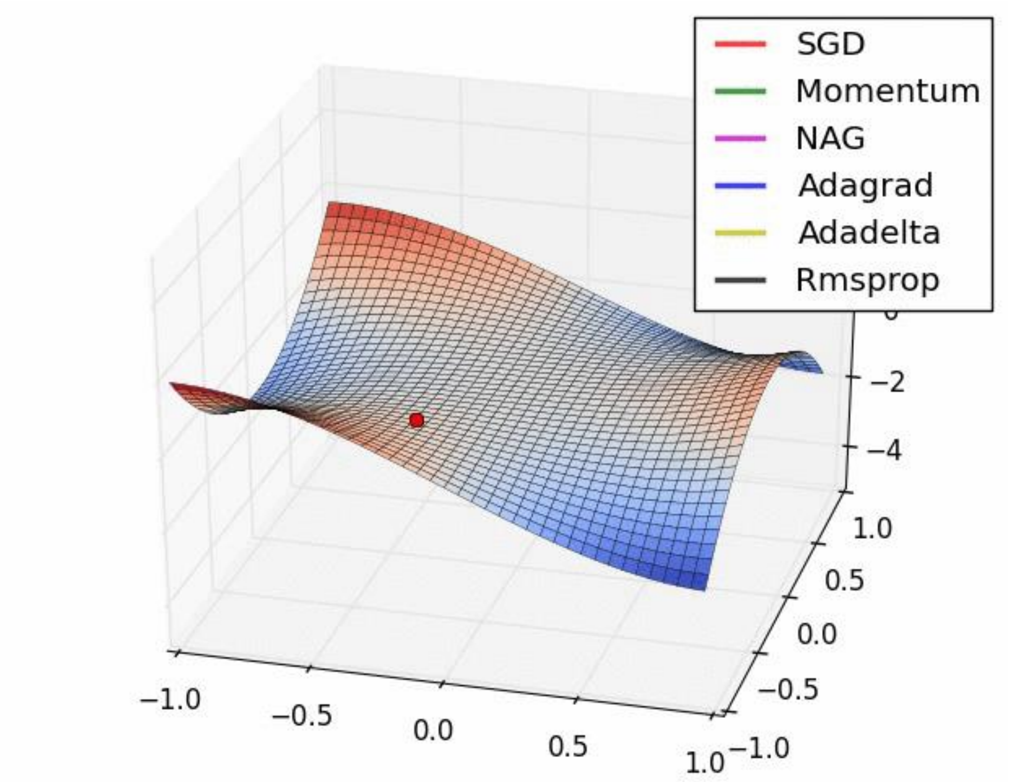
β is a hyperparameter controlling amount of momentum
$\delta\theta(t)$ is the previous weight change





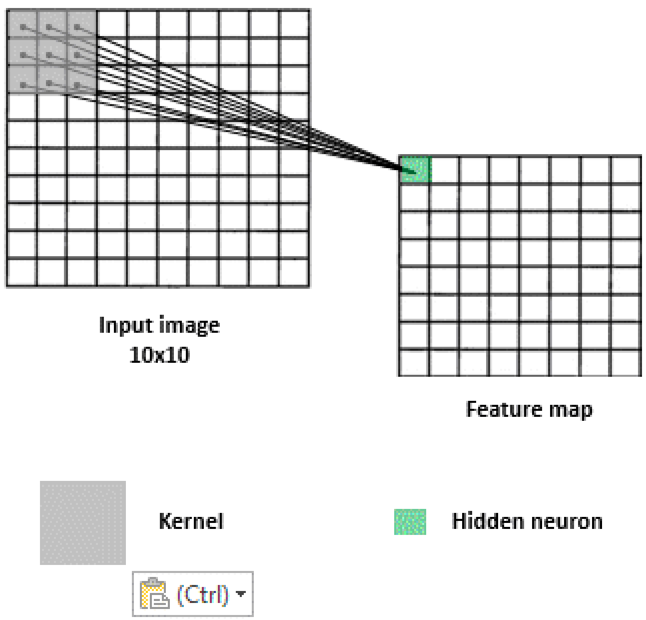
Implementation: optimisers

- There are many different optimisers that can be used instead of GD and momentum
  - Often adapting learning rates



Images: shared weights

- Consider an image:
  - 1M pixels
  - 10k neurons on first hidden layer
  - = 10,000,000,000 weights to first layer!!!!
- Instead of connecting everything, connect small local patches (kernels)
  - Share weights between all patches
  - Far fewer weights!
  - Asking hidden neuron to activate wherever this pattern is seen



- Define many of these patches
- Called: convolutional neural network
  - Main architecture for images

Recap

- Recap on neural networks
- Revisited the perceptron learning rule
- General idea of learning
- Forward propagation
- Backpropagation
- Incorporating gradient descent
- Tips for improving training
    - Initialisation, normalisation, dropout, momentum, optimisers, shared weights