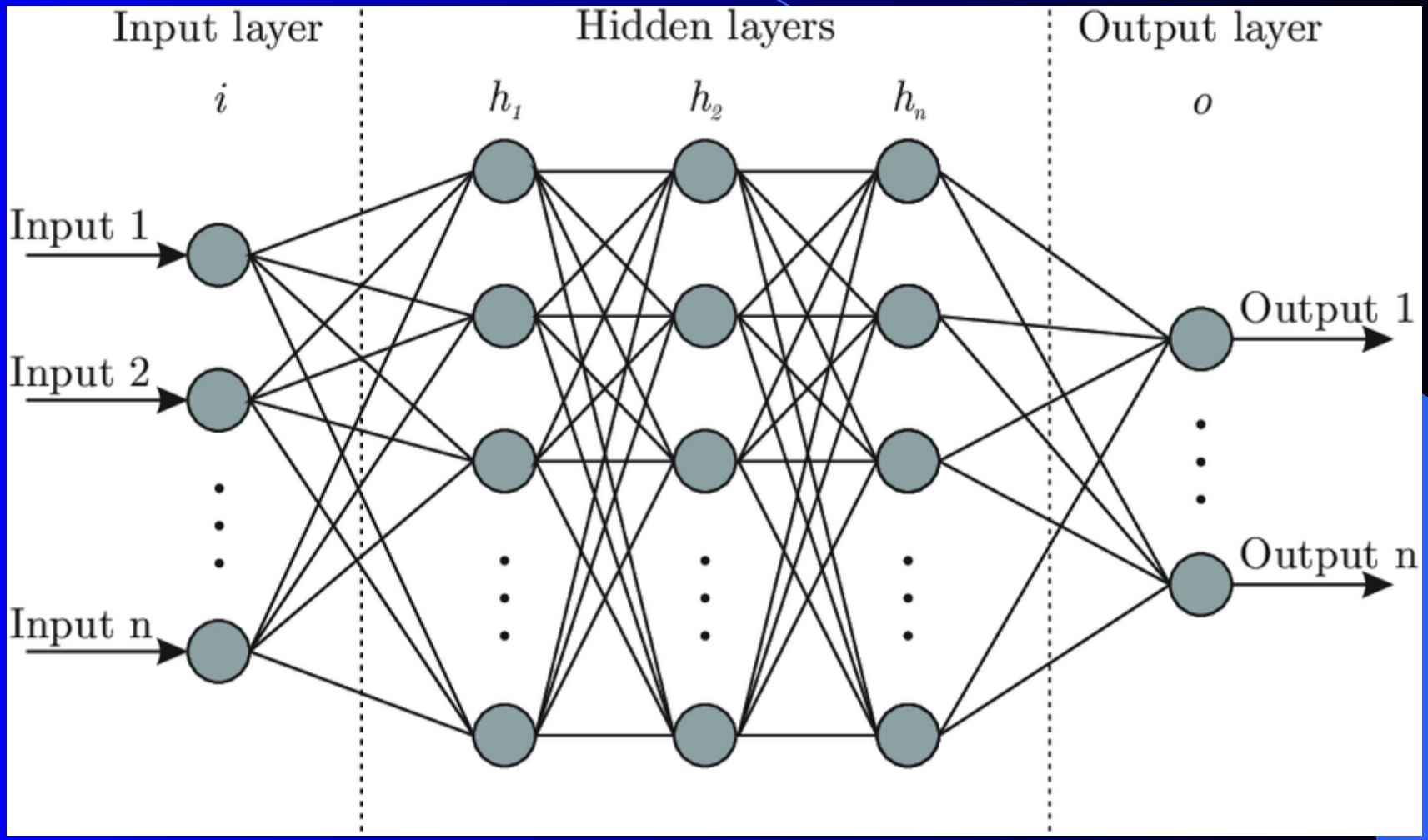
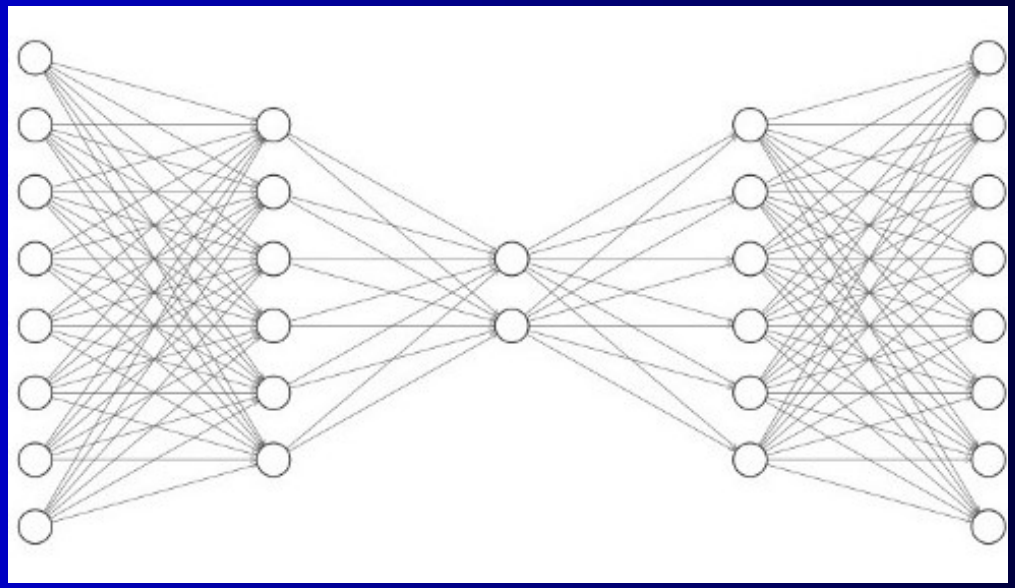
Multi-layer Perceptron with Backpropagation Learning

Multi-layer Perceptron (MLP)



What are the Hidden Nodes Doing?

- Higher order features vs 1st order features (perceptron/Us)
  - The real power of machine learning (exponential # of variations)
- Hidden nodes discover new *higher order* features which are fed into subsequent layers



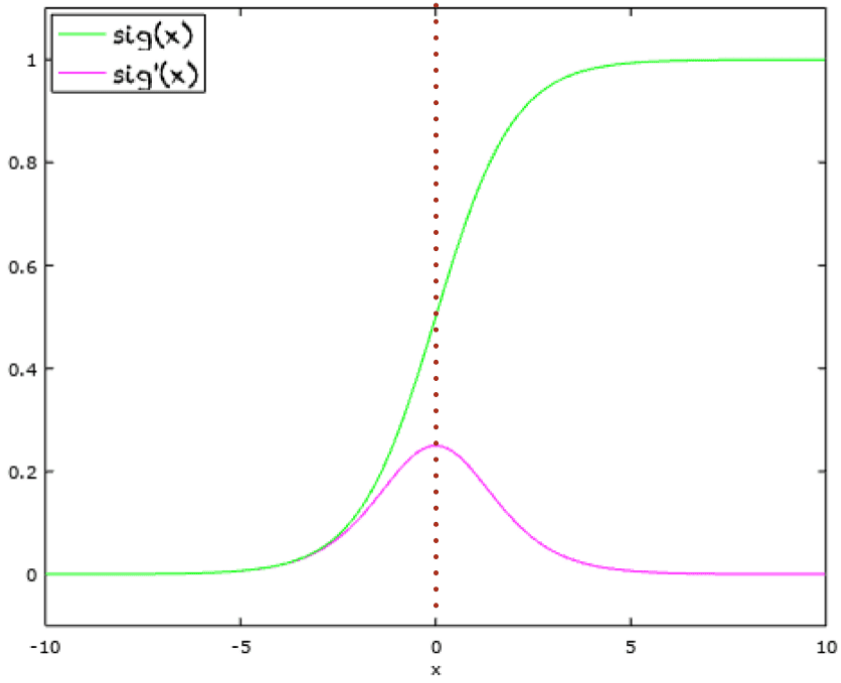
Number of Hidden Nodes

- How many needed is a function of how hard the task is
- Common to use one fully connected hidden layer. Initial number could be ~2n hidden nodes where n is the number of inputs.
- In practice we train with a small number of hidden nodes, then keep doubling, etc. until no more significant improvement on test sets
  - Too few will underfit
  - Too many nodes can make learning slower and could overfit
    - Having somewhat too many hidden nodes is preferable if using reasonable regularization; avoids underfit and should ignore unneeded nodes
- Each output and hidden node should have its own bias weight

NON-LINEAR ACTIVATIONS

Sigmoid Function

- Differentiable, most unstable in middle



Plot of σ(x) and its derivate σ'(x)

Domain: (−∞, +∞)

Range: (0, +1)

σ(0) = 0.5

Other properties

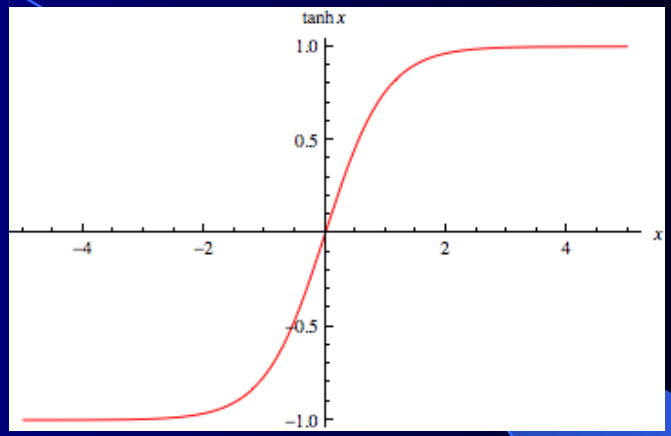
$$\sigma(x) = 1 - \sigma(-x)$$

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

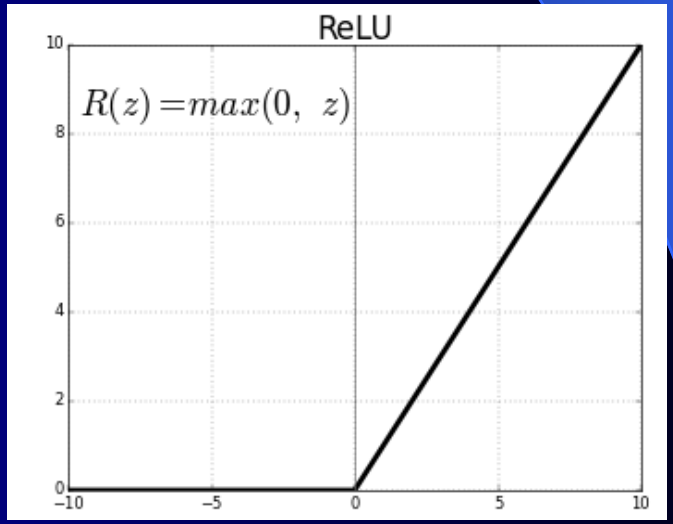
$$\sigma'(x) = \sigma(x)(1-\sigma(x))$$

Other Activation Functions

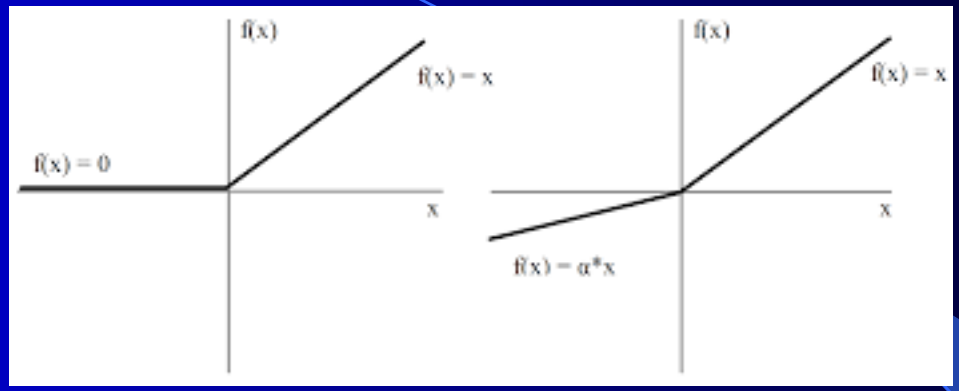
- Hyperbolic tangent (tanh)
  - Same shape as sigmoid but tanh(0)=0 (rather than 0.5)



- Rectified linear activation function (ReLU)
  - Popular in deep nets



Rectified Linear Units



- BP can work with any differentiable non-linear activation function (e.g. sine)
- *ReLU* is common these days especially with deep learning: $f(x) = \text{Max}(0,x)$
  - More efficient computation: Only comparison, addition and multiplication
  - $f'(net)$ is 0 or constant, just fold into learning rate
- Leaky ReLU $f(x) = x$ if $x > 0$, else ax, where $0 \leq a <= 1$, so for net < 0 the derivate is not 0 and can do some learning (does not "die").
  - Lots of other variations
- Sparse activation: For example, in a randomly initialized networks, only about 50% of hidden units are activated (having a non-zero output)
- Not differentiable but we just "cheat" and include the discontinuity point with either side of the linear part of the ReLU function – piecewise linear

Regression with MLP/BP

- For regression in MLPs we use the sum-squared error (L2) loss. More natural for regression than for classification.
- Output nodes use a linear activation (i.e. identity function which just passes the *net* value through). This naturally supports unconstrained regression.
  - Don't typically normalize output
- The output error is still $(t - z) f'(net)$, but since $f'(net)$ is 1 for the linear activation, the output error is just (*target* – *output*)
- Hidden nodes still use a non-linear activation function (such as logistic) with the standard $f'(net)$
- This is how sklearn always does MLP regression

Softmax Output Layer Activation

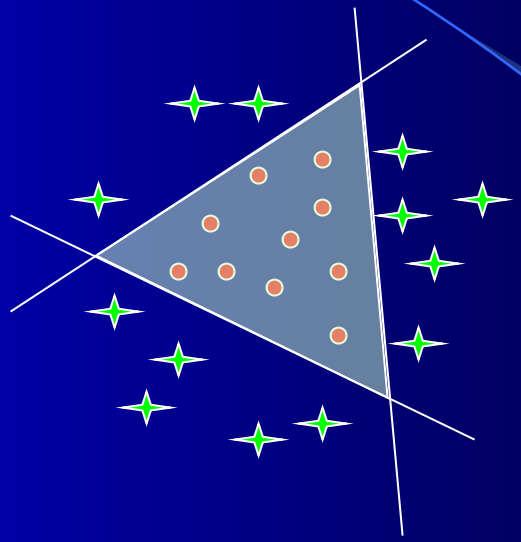
- For *classification* problems it is increasingly popular to use the *softmax* activation function, just at the output layer
- Softmax (softens) 1 of *n* targets to mimic a probability vector for the output nodes
- If there were 3 output nodes with net values 0, .5, and 1 then the outputs for each node would be .18, .31, .51 which sums to 1 and can be considered as probability estimates
- All the hidden nodes still do a standard activation function such as logistic, hyperbolic tangent, or ReLU
- Sklearn automatically uses softmax at the output layer for MLP classification, and you choose the activation function for hidden nodes

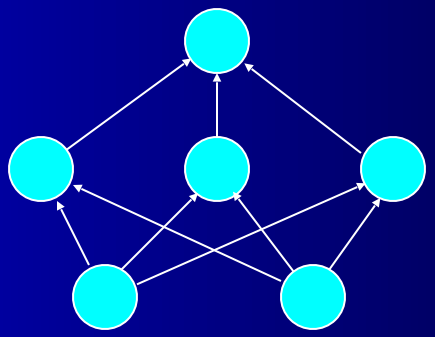
Cross-Entropy and Softmax

- For *classification* it is increasingly popular to use the cross-entropy loss function.
- Cross entropy measures the difference (in entropy) between two distributions.
- We must recalculate the gradient weight update equation when we use new activation/ loss functions.
- The hidden layers still update as usual and include $f'(net)$
- Sklearn always uses this approach for MLP classification

t	z	CE
0	0	0
1	1	0
1	.9	.11
1	.5	.69
1	.1	2.30

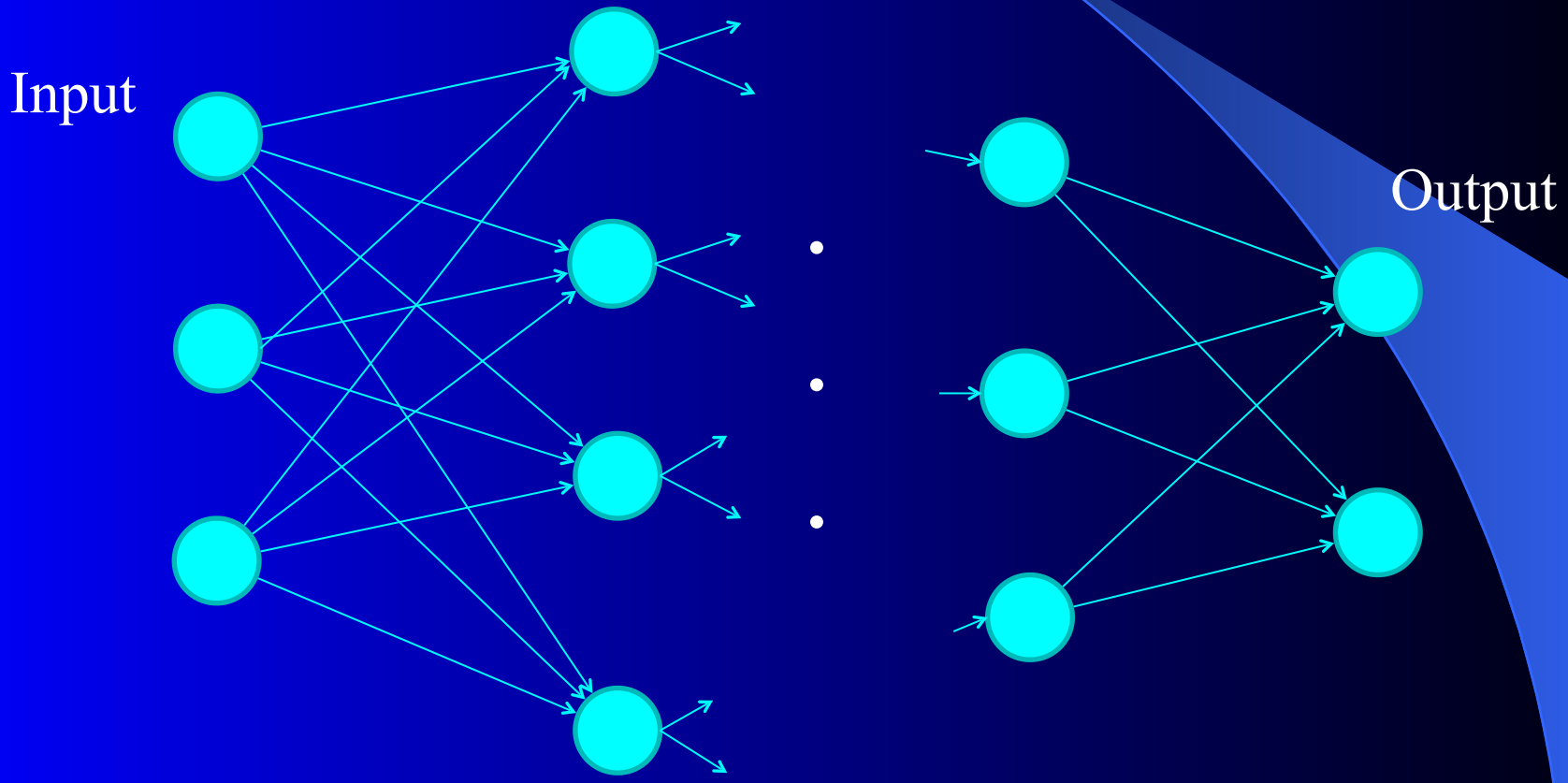
Multi-Layer Generalization





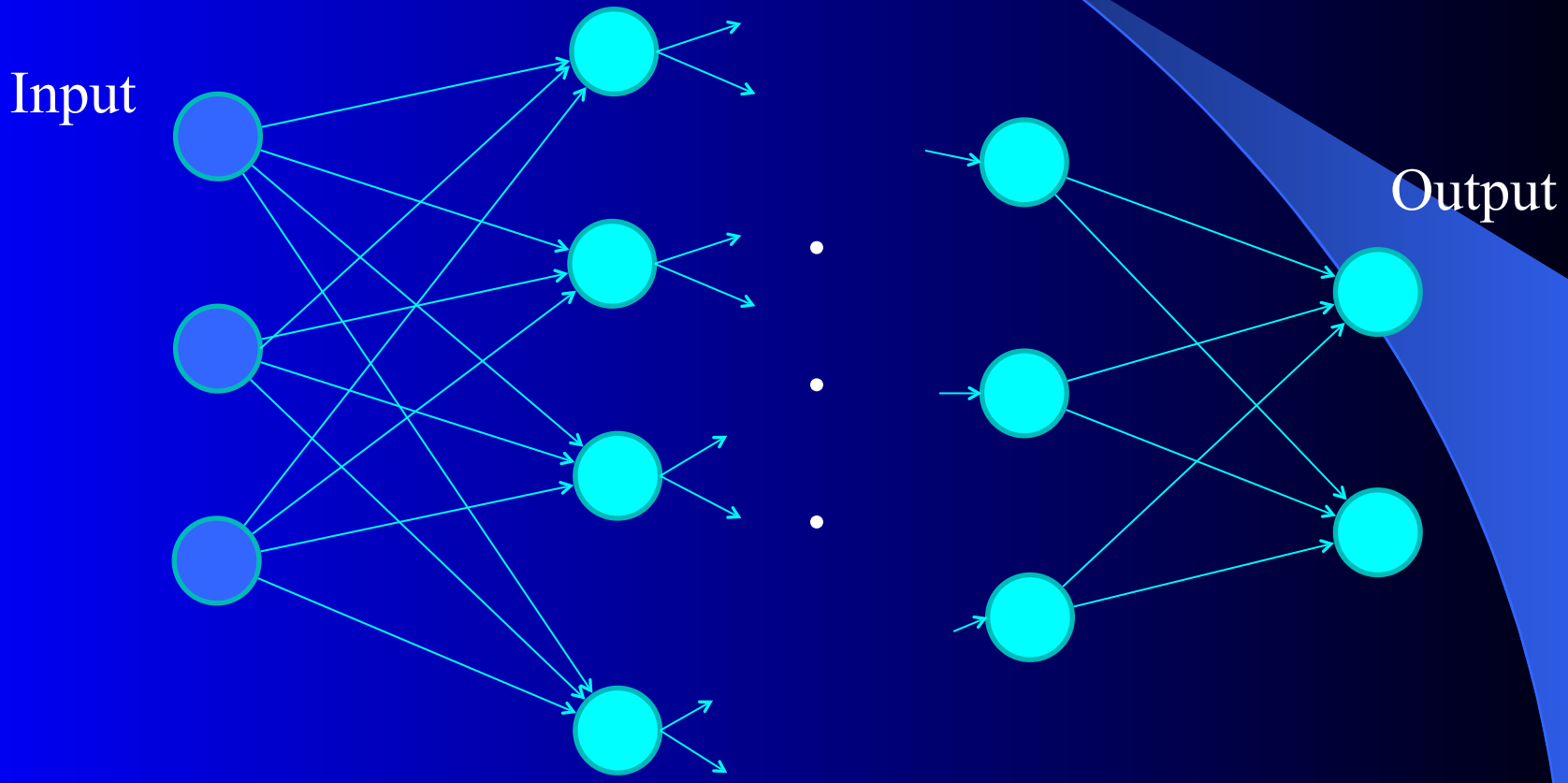
Back-Propagation

- Operates similarly to perceptron learning



Back-Propagation

- Inputs are fed forward through the network



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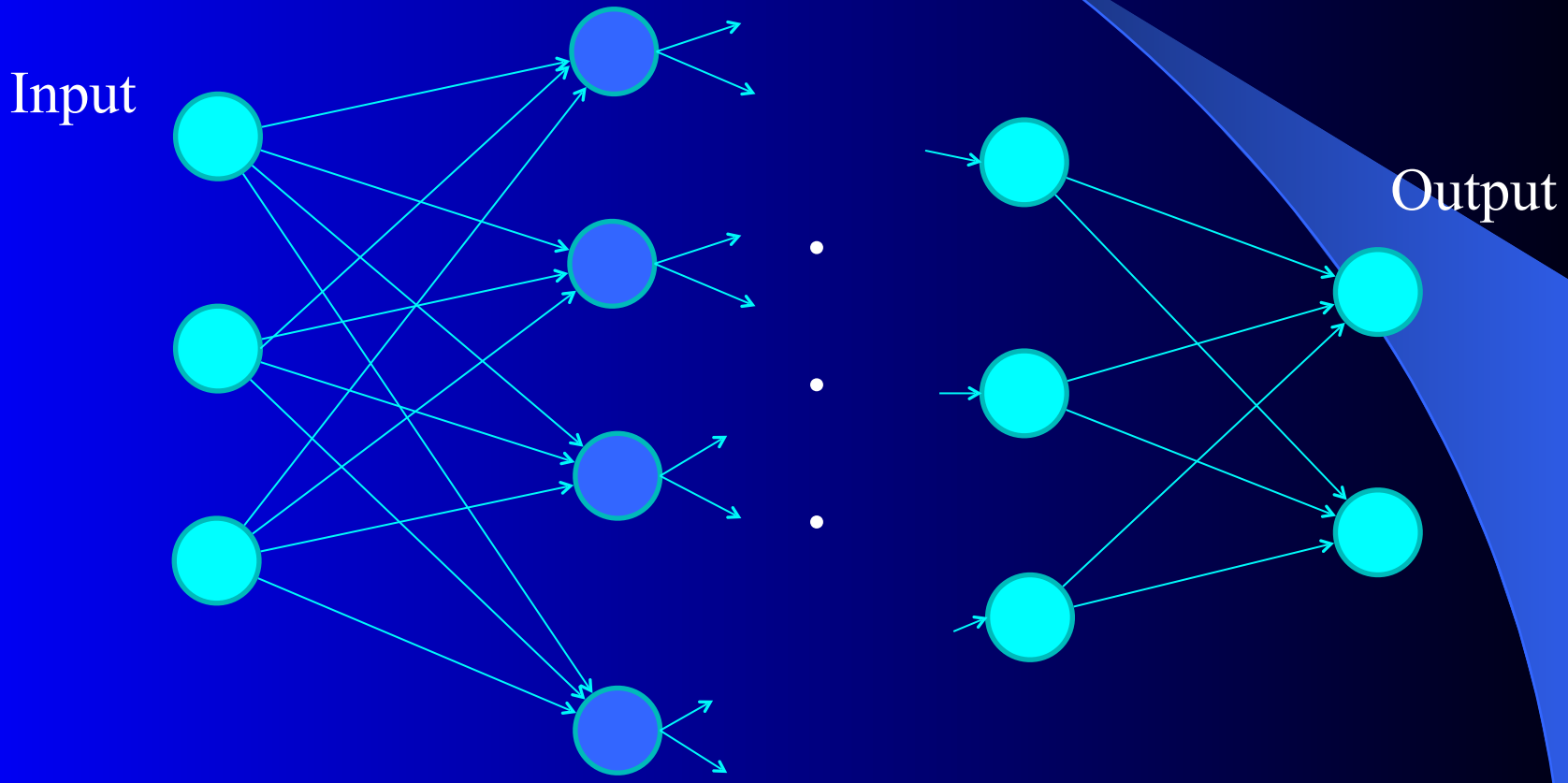

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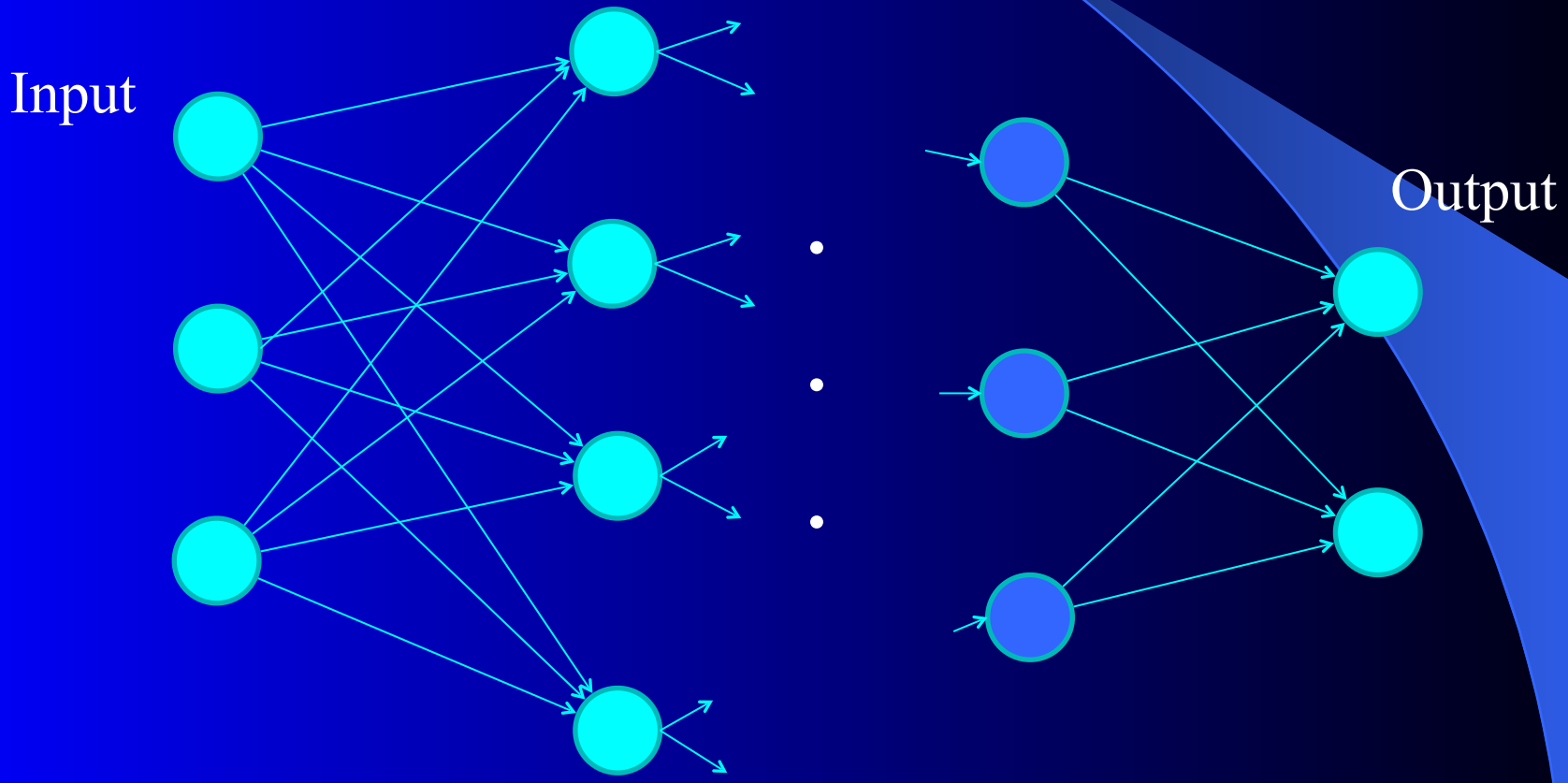

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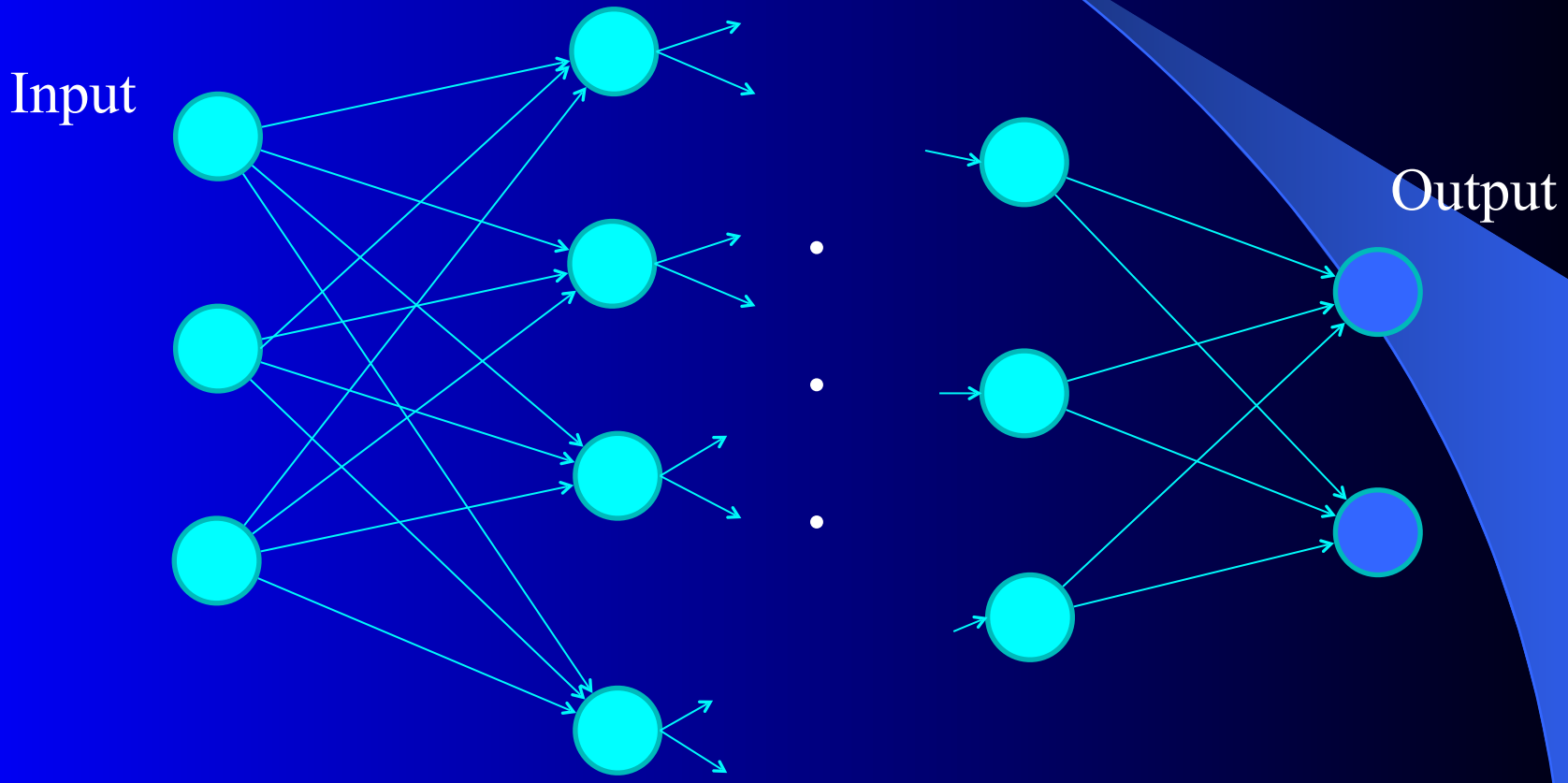

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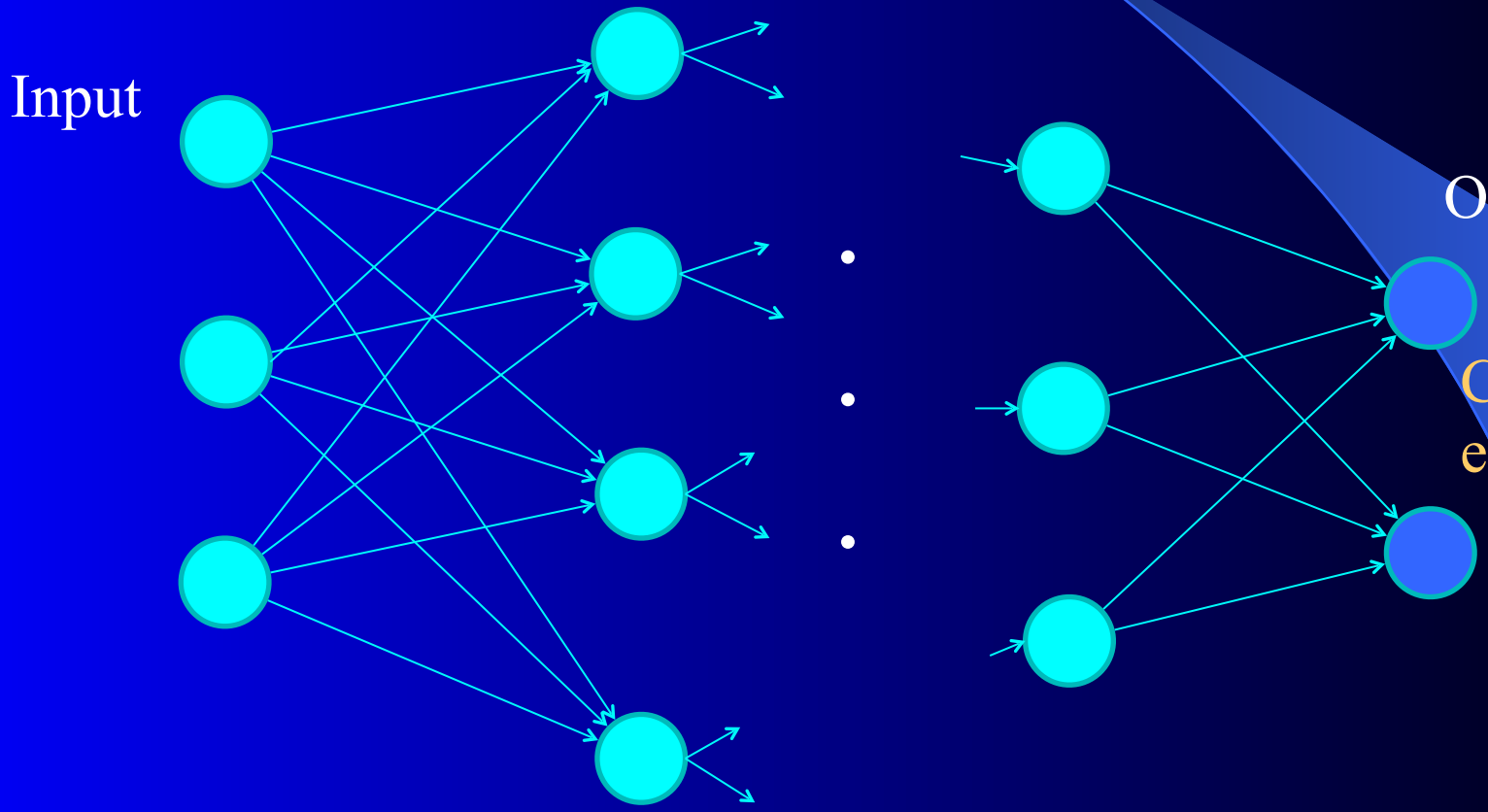
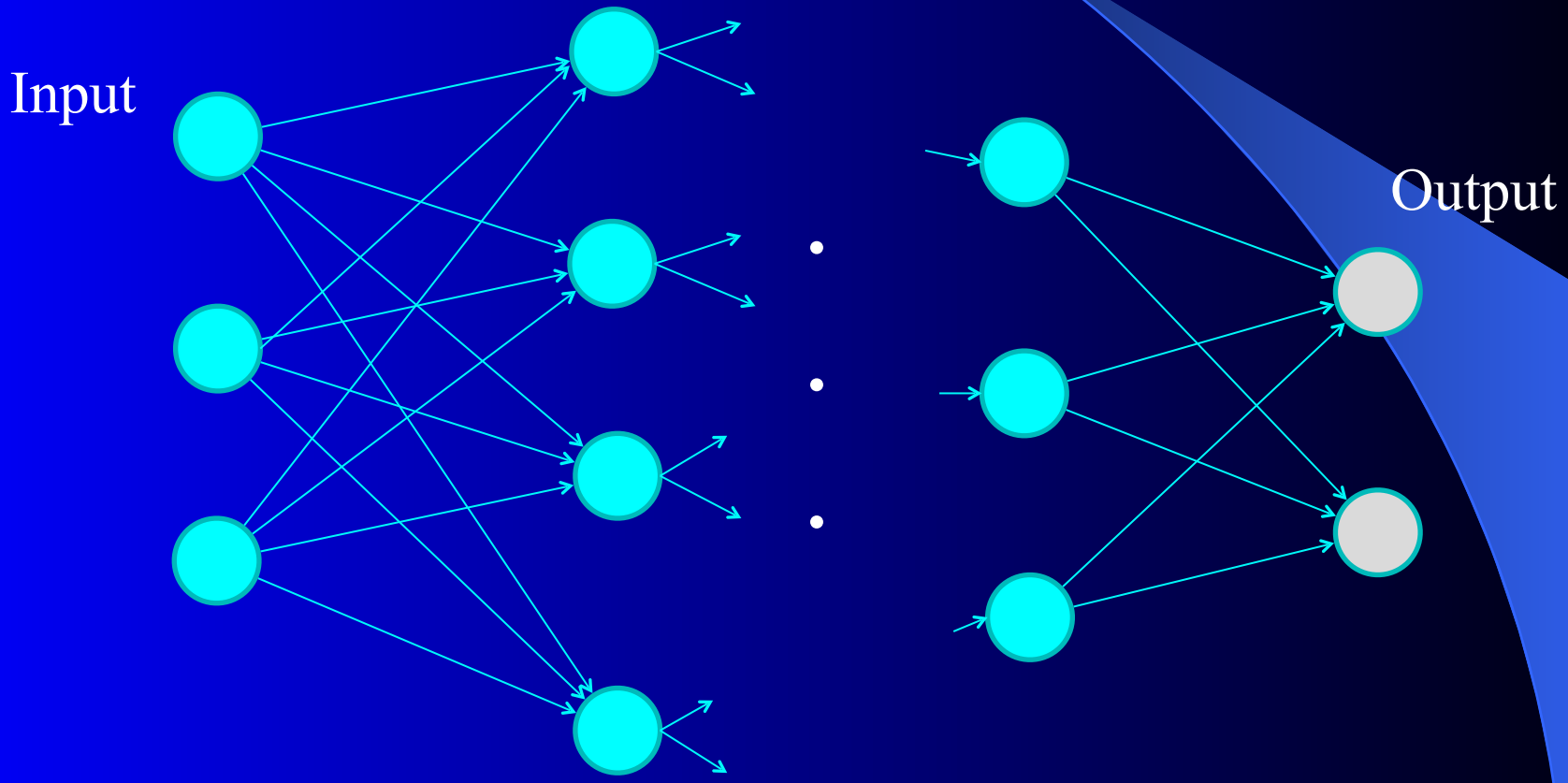


Back-Propagation

- Errors are propagated back



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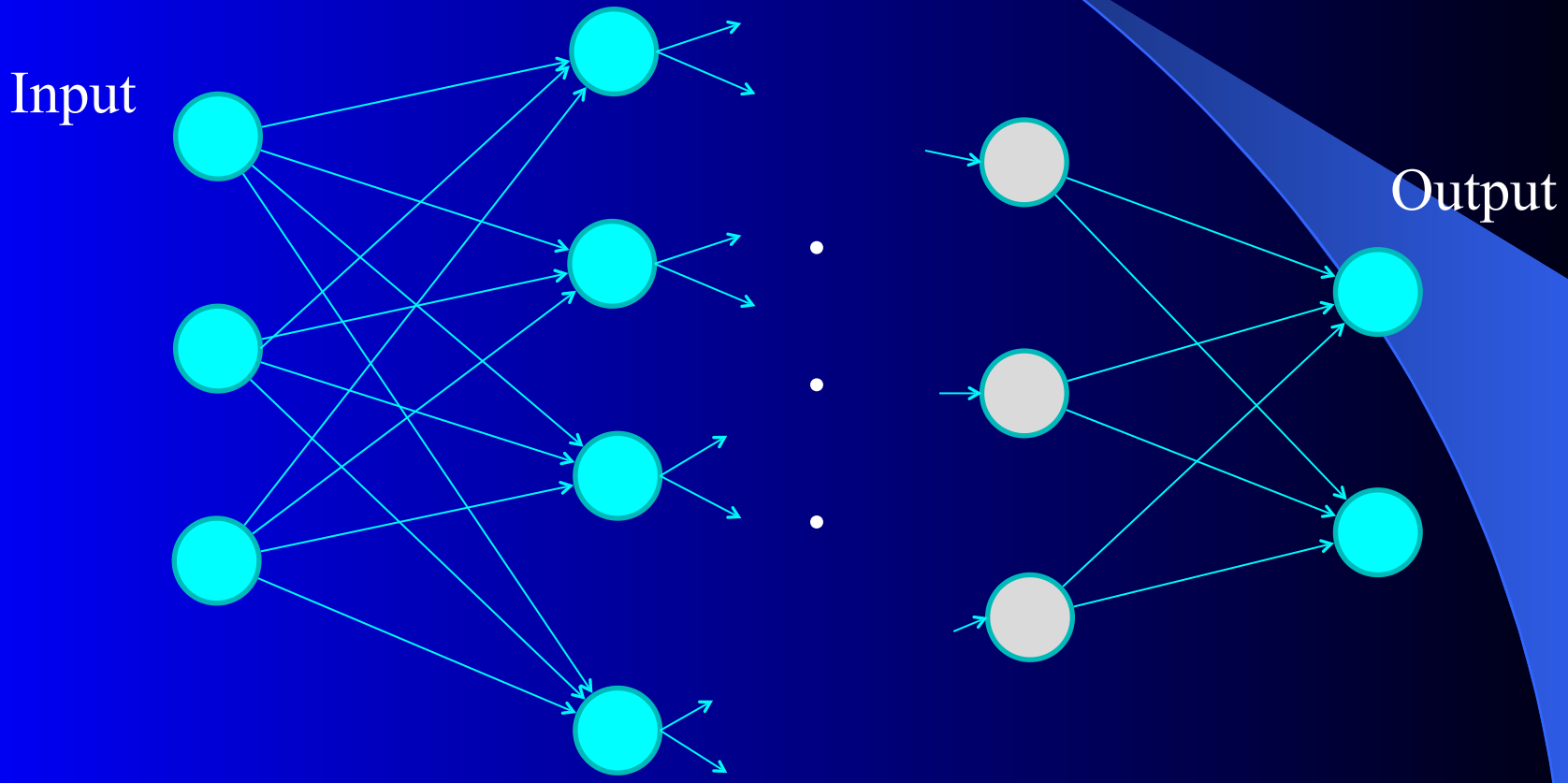

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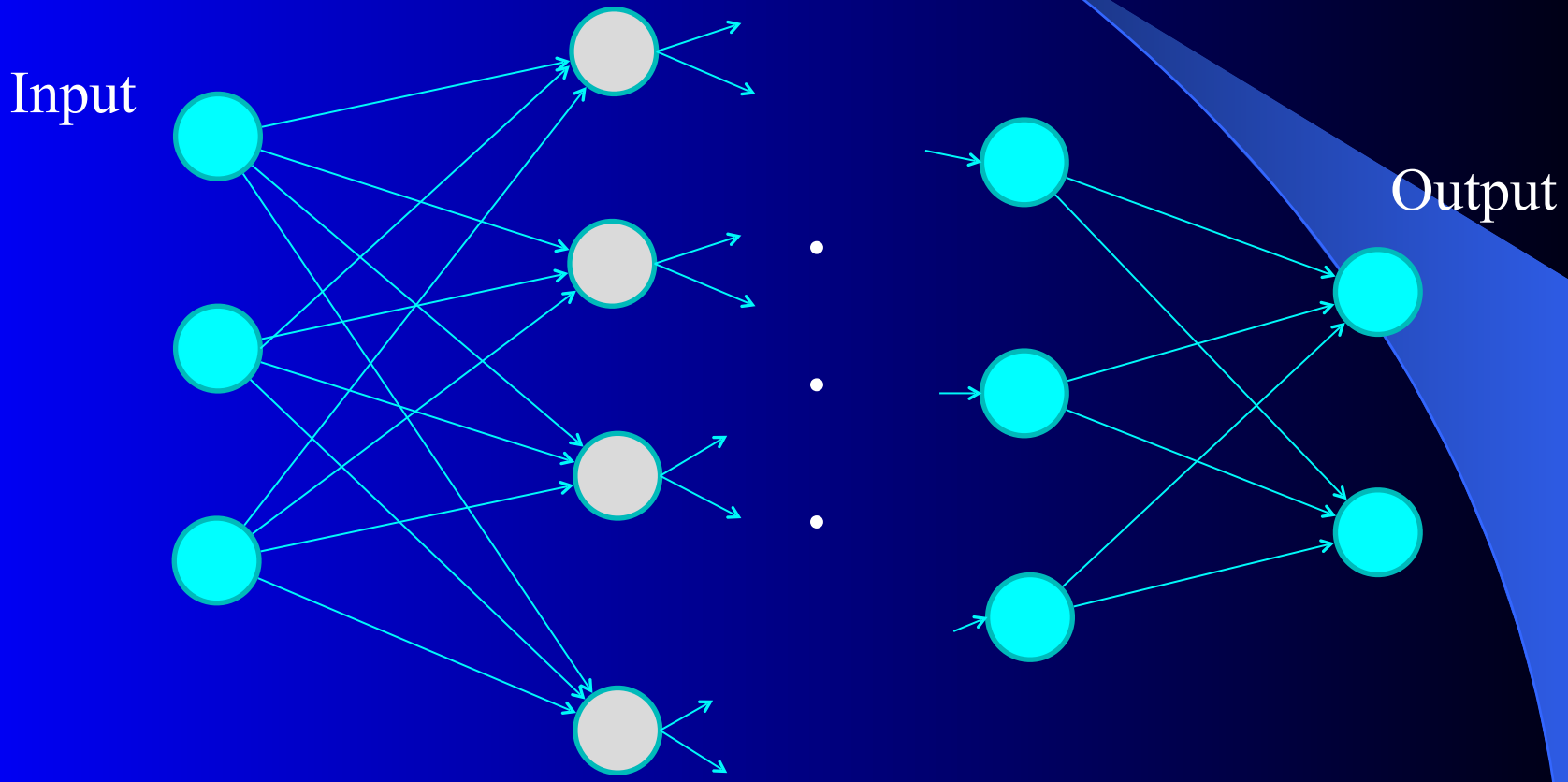

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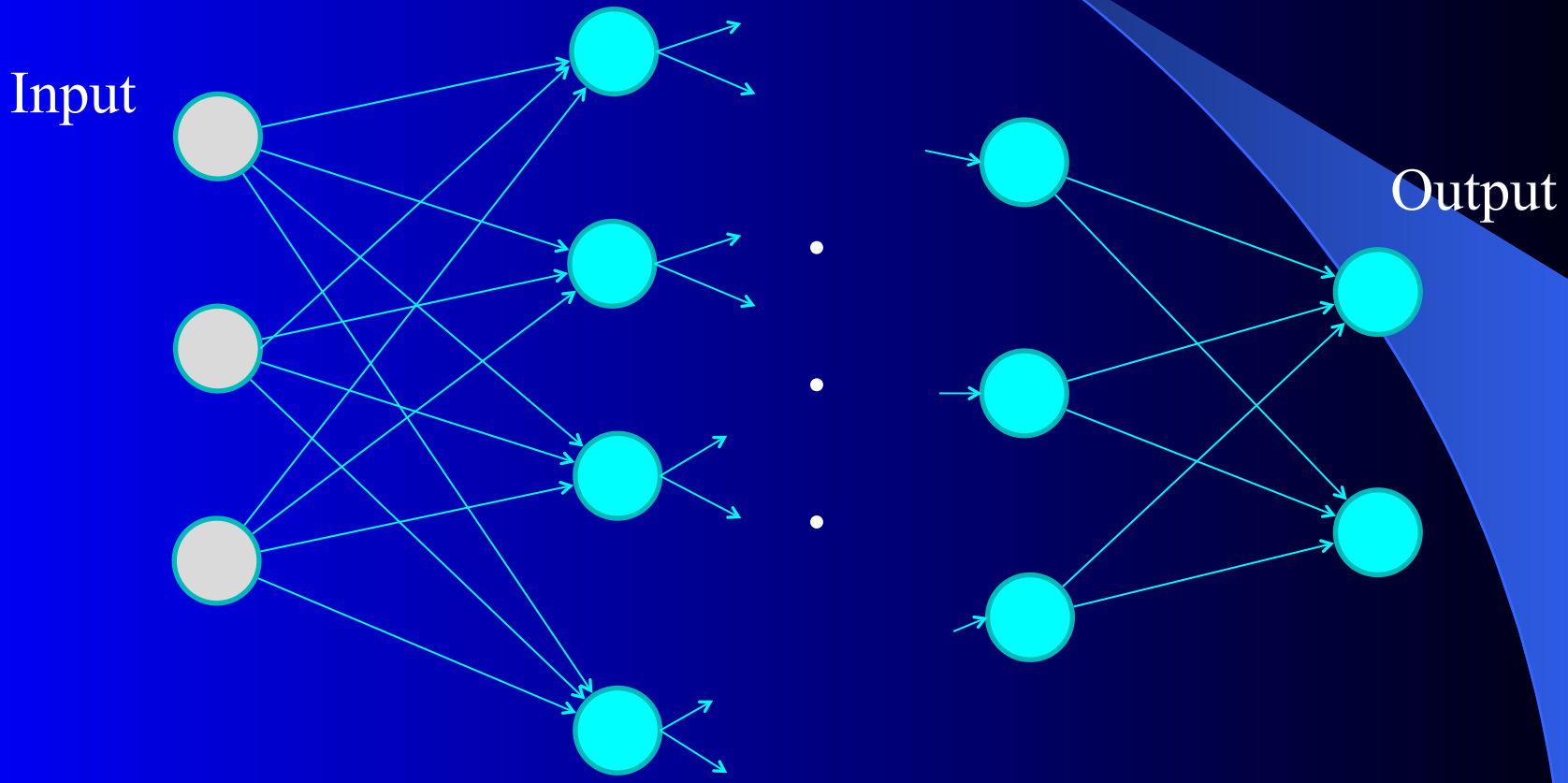
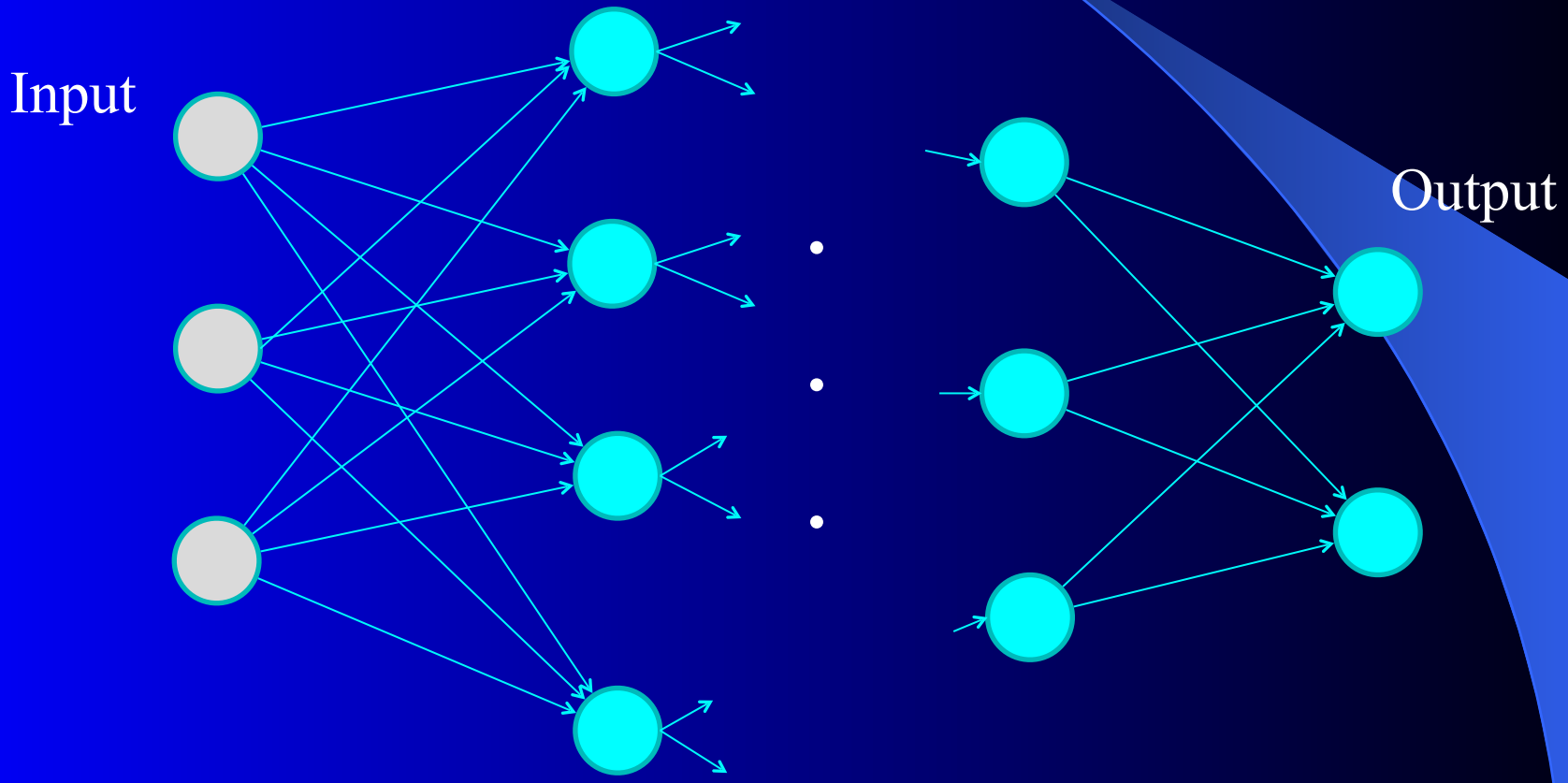


Back-Propagation

- Adjust weights based on errors



Back-Propagation Training

- Weights might be updated after each pass or after multiple passes
- Need a comprehensive training set
- Network cannot be too large for the training set
- No guarantees the network will learn
- Network design and learning strategies impact the speed and effectiveness of learning

Batch Update

- With On-line (stochastic) update we update weights after every instance
- With Batch update we accumulate the changes for each weight, but do not update them until the end of each epoch
- Batch update gives a correct direction of the gradient for the entire data set, while on-line could do some weight updates in directions quite different from the average gradient of the entire data set
  - Based on noisy instances and also just that specific instances will not usually be at the average gradient
- Proper approach? - Conference experience/Parallel experience
  - Most (including us) assumed batch more appropriate, but batch/on-line a non-critical decision with similar results
- We show that batch is less efficient
  - Wilson, D. R. and Martinez, T. R., The General Inefficiency of Batch Training for Gradient Descent Learning, *Neural Networks*, vol. **16**, no. 10, pp. 1429-1452, 2003

Speed up variations of SGD

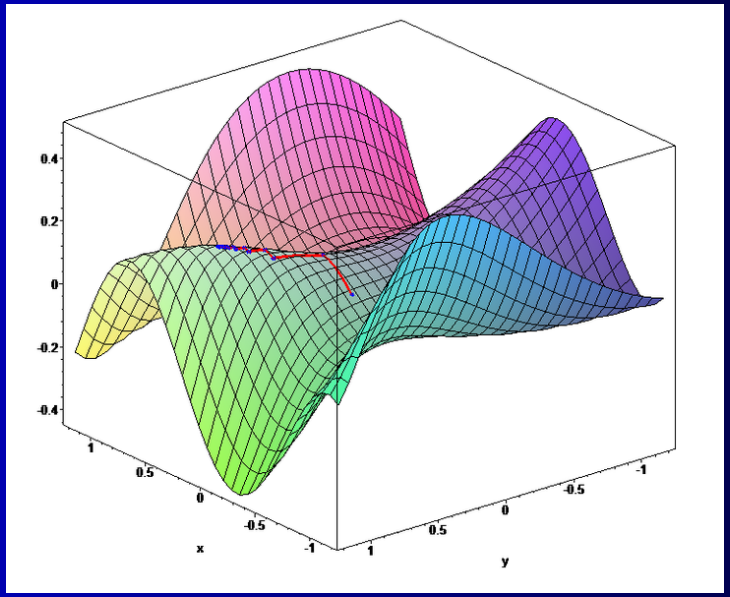
- Use mini-batch rather than single instance for better gradient estimate – *Sometimes* helpful if SGD variation more sensitive to bad gradient, and also for some parallel (GPU) implementations.

- Adaptive learning rate approaches (and other speed-ups) are often used for deep learning since there are so many training updates
  - Standard Momentum
    - Note that these approaches already do an averaging of gradient, also making mini-batch less critical
  - Nesterov Momentum – Calculate point you would go to if using normal momentum. Then, compute gradient at that point. Do normal update using *that* gradient and momentum.
  - Rprop – Resilient BP, if gradient sign inverts, decrease it's individual LR, else increase it – common goal is faster in the flats, variants that backtrack a step, etc.
  - Adagrad – Scale LRs inversely proportional to sqrt(sum(historical values))
  - RMSprop – Adagrad but uses exponentially weighted moving average, older updates basically forgotten
  - Adam (Adaptive moments) –Momentum terms on both gradient and squared gradient (uncentered variance) (1st and 2nd moments) – updates based on a moving average of both - Popular

Local Minima and Neural Networks

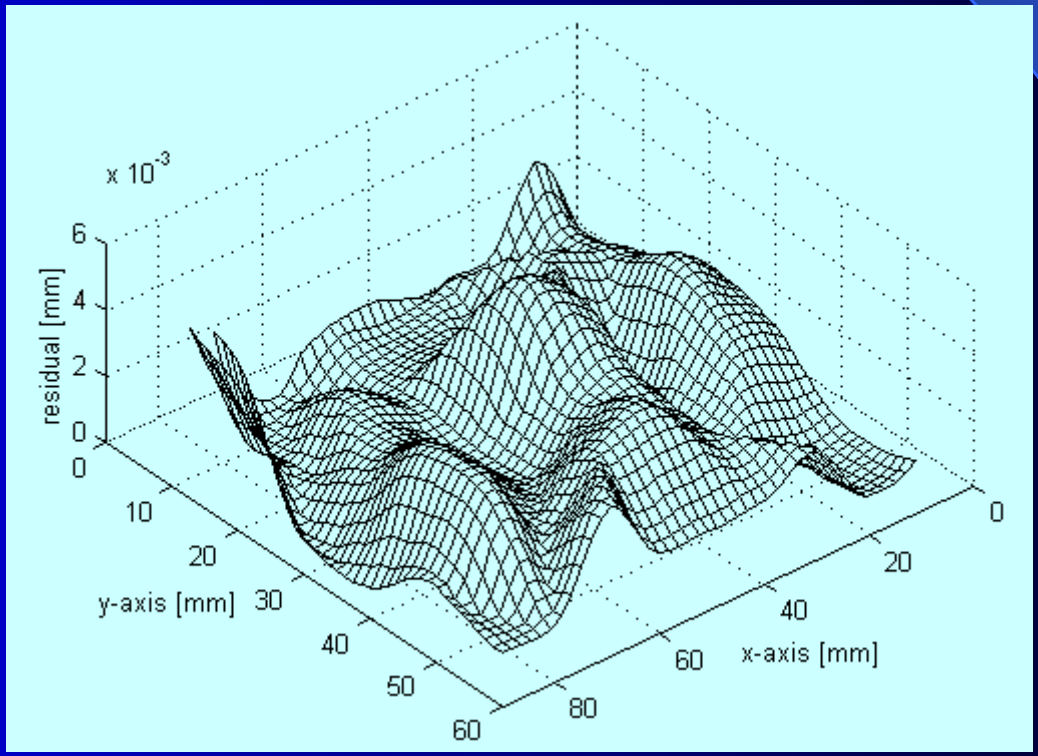
- Neural Network can get stuck in local minima for small networks, but for most large networks (many weights), local minima rarely occur in practice

- This is because with so many dimensions of weights it is unlikely that we are in a minima in every dimension simultaneously – almost always a way down



Learning Rate

- Learning Rate - Relatively small (.01 - .5 common), if too large BP will not converge or be less accurate, if too small it is just slower with no accuracy improvement as it gets even smaller.



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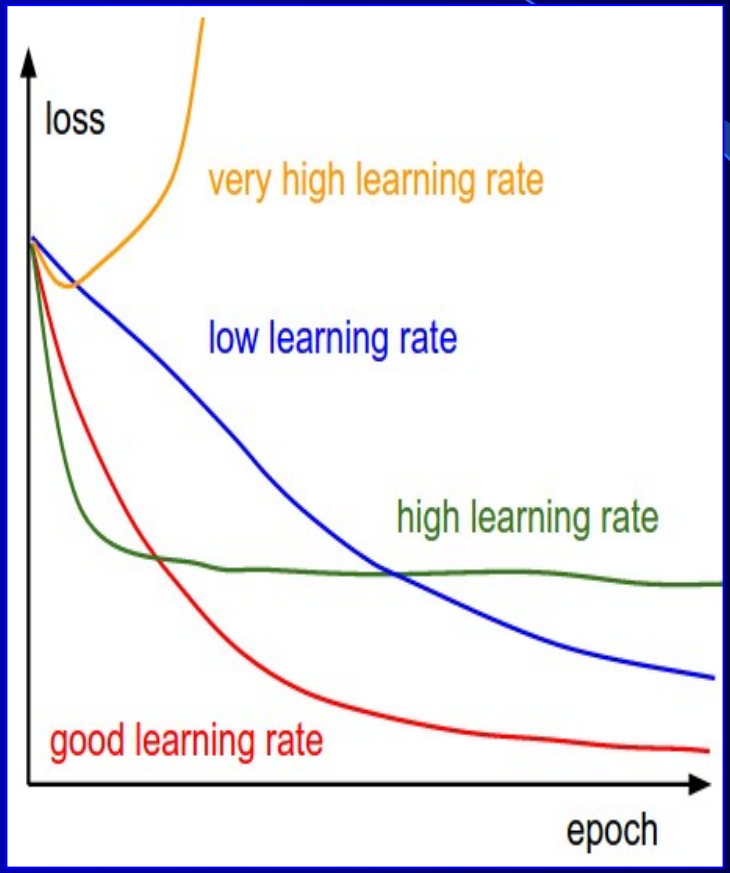
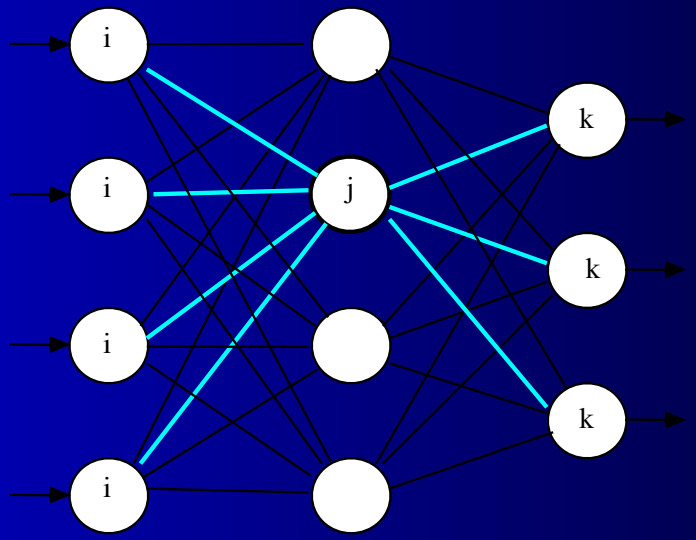


Backpropagation Learning Algorithm

- Until Convergence (low error or other stopping criteria) do
  - Present a training instance
  - Calculate the error of the output nodes (based on $T - Z$)
  - Calculate the error of the hidden nodes (based on the error of the output nodes which is propagated back to the hidden nodes)
  - Continue propagating error back until the input layer is reached
  - Then update all weights based on the standard delta rule with the appropriate error function
- No bias δ:
  - Note that you never have to calculate δ for a bias node since no layers before the bias node have nodes connected to it.
  - You update the bias node weight based only on the nodes that follow the bias, i.e., are connected to the bias after it.

Backpropagation Learning Equations



Error Computation

Let p and q be two units connected to each other in a feedforward neural network, such that q follows p. Let δ_q denote the error at q.

If q is in the **output** layer,

$$\delta_q = (t_q - o_q)o_q(1 - o_q)$$

If q is in a **hidden** layer,

$$\delta_q = (\sum_{k \in follows(q)} w_{qk}\delta_k)o_q(1 - o_q)$$

It follows that:

$$\Delta w_{pq} = c\delta_q o_p$$

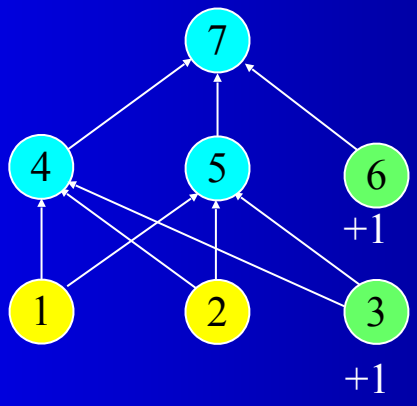
Note that $o_q\left(1 - o_q\right)$ is the derivative – dampens where "certain", enhances where "uncertain"

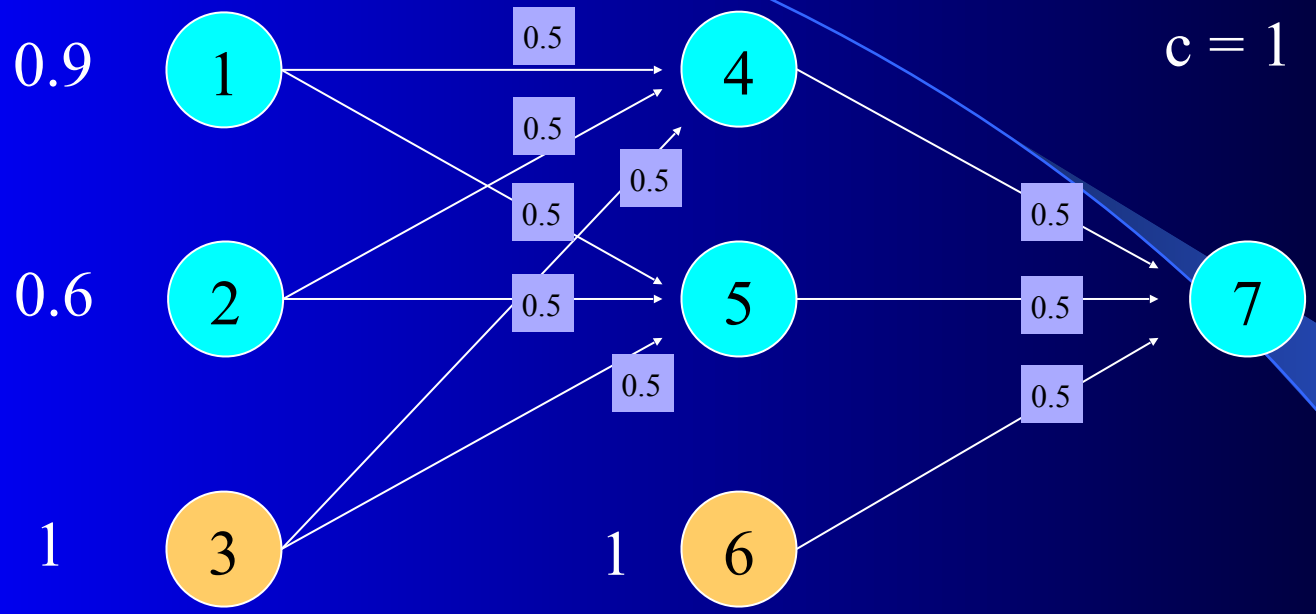
Also note that o_p is the output of node p – we often refer to it as z_p

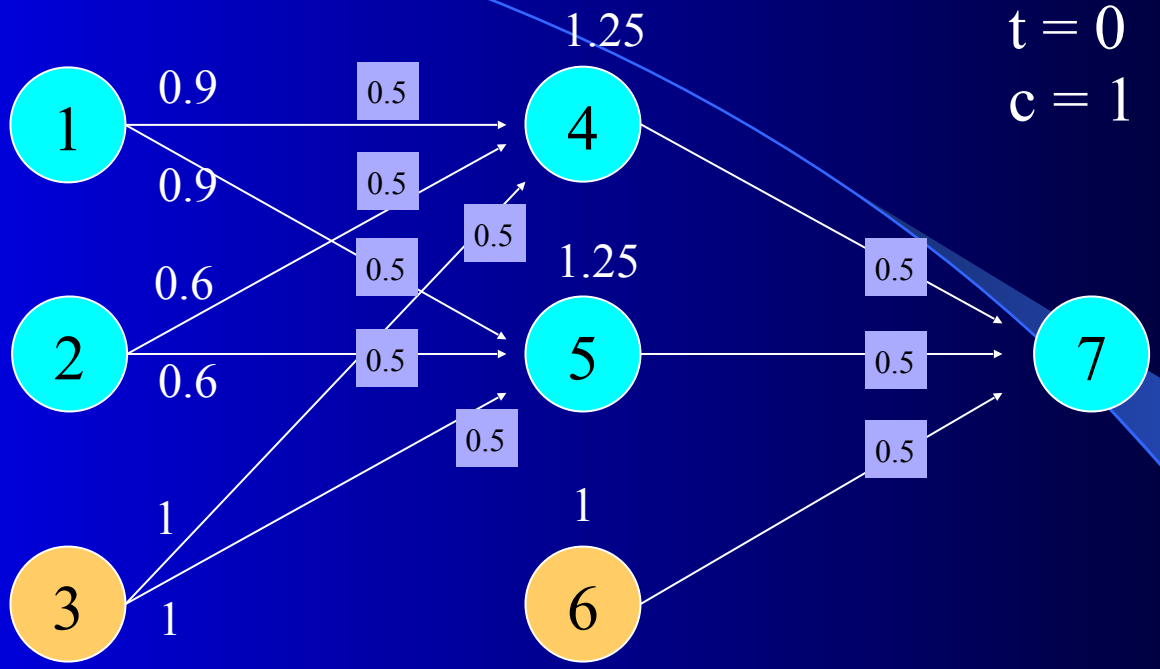
Backpropagation Learning Example

Assume the following 2-2-1 MLP has all weights initialized to .5. Assume a learning rate of 1. Show the updated weights after training on the data .9 .6 ==> 0.

Show all net values, activations, outputs, and errors. Nodes 1 and 2 (input nodes) and 3 and 6 (bias inputs) are just placeholder nodes and do not pass their values through an activation.



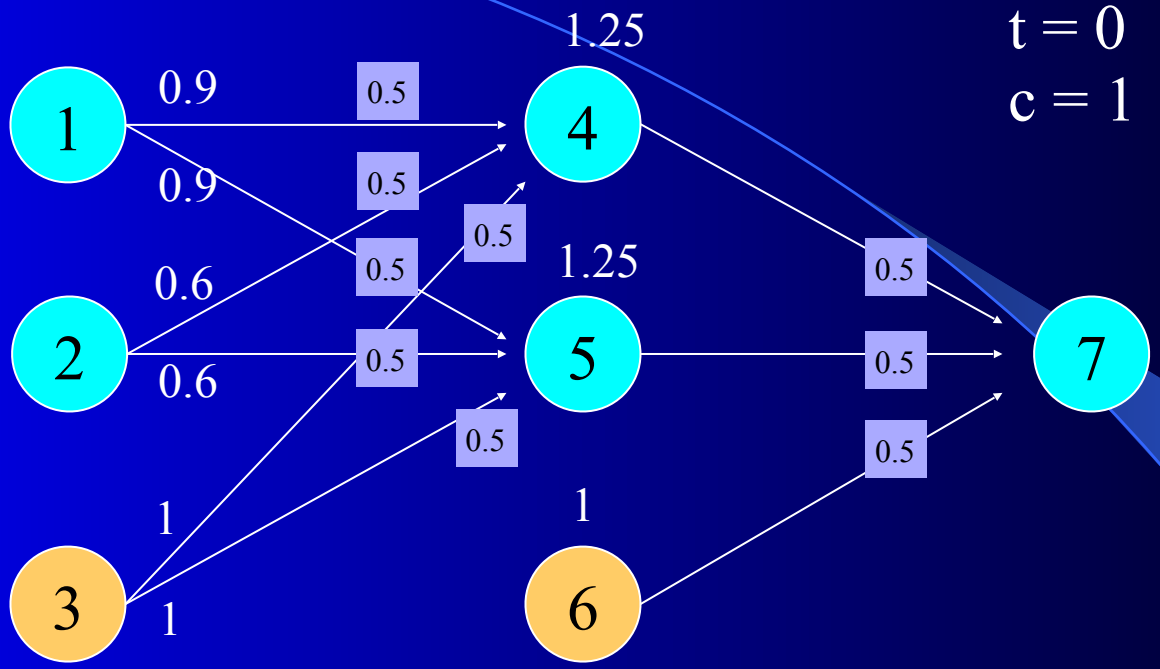

0.5 Weights
t = 0
c = 1 # Learning Rate
0.9
0.6
1
1
1
2
3
4
5
6
7
0.5
0.5
0.5
0.5
0.5
0.5
0.5
0.5
0.5



$$net_q = \sum_{i=1}^{3} x_i w_{ij}$$

$net_4 = .9 * .5 + .6 * .5 + 1 * .5 = 1.25$

$net_5 = 1.25$



$$net_q = \sum_{i=1}^{3} x_i w_{ij}$$

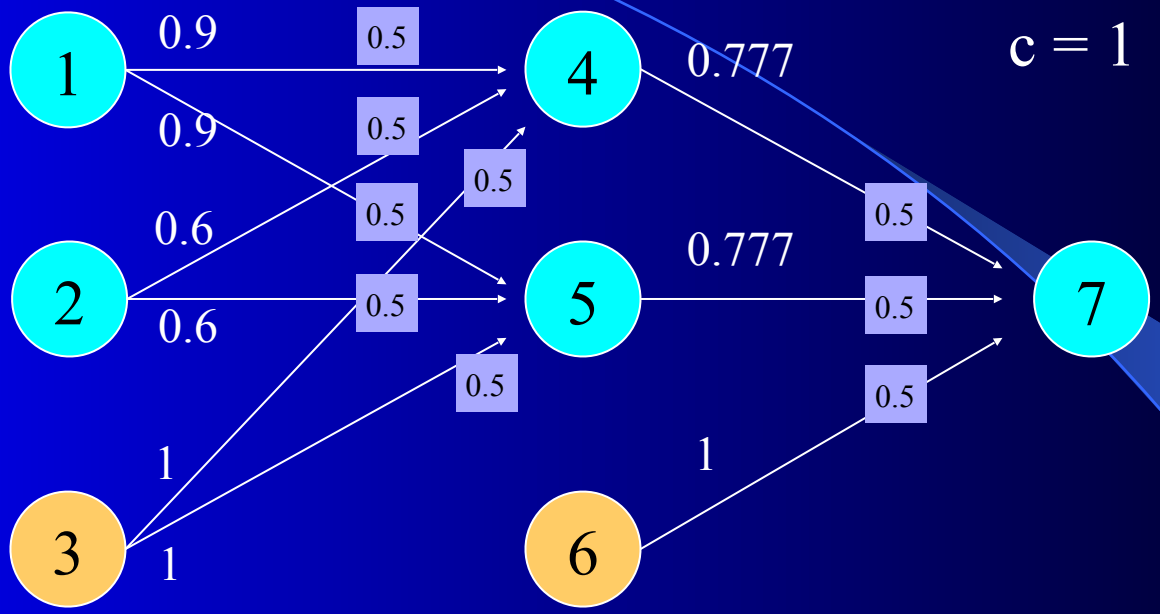
$$z_i = \frac{1}{1 + e^{-net_i}}$$

$net_4 = .9 * .5 + .6 * .5 + 1 * .5 = 1.25$

$net_5 = 1.25$

$z_4 = 1/(1 + e^{-1.25}) = .777$

$z_5 = .777$



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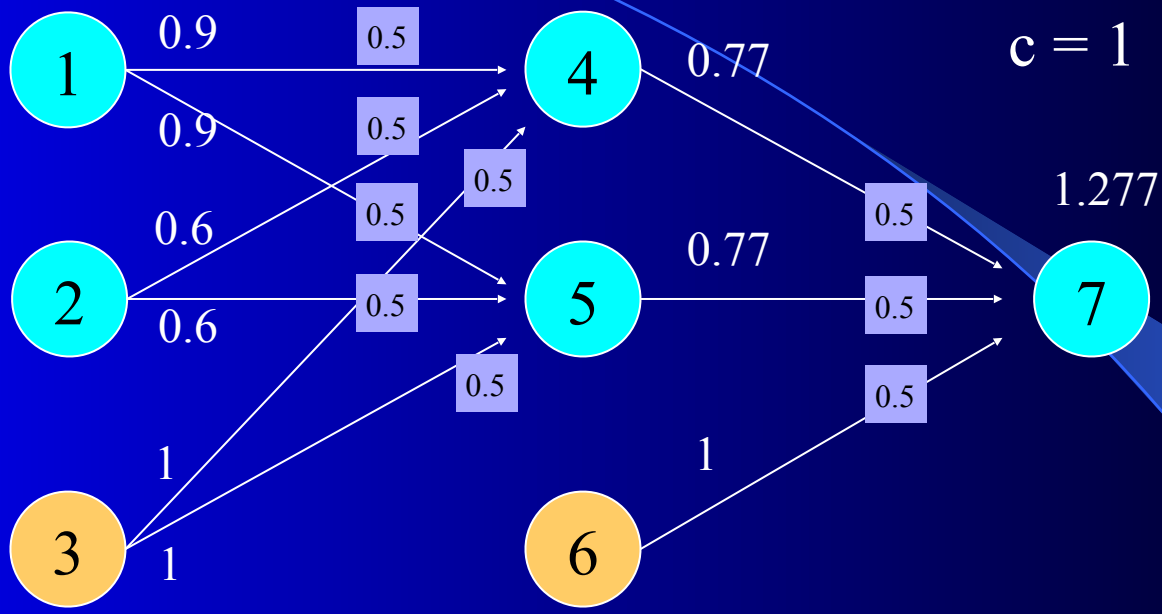

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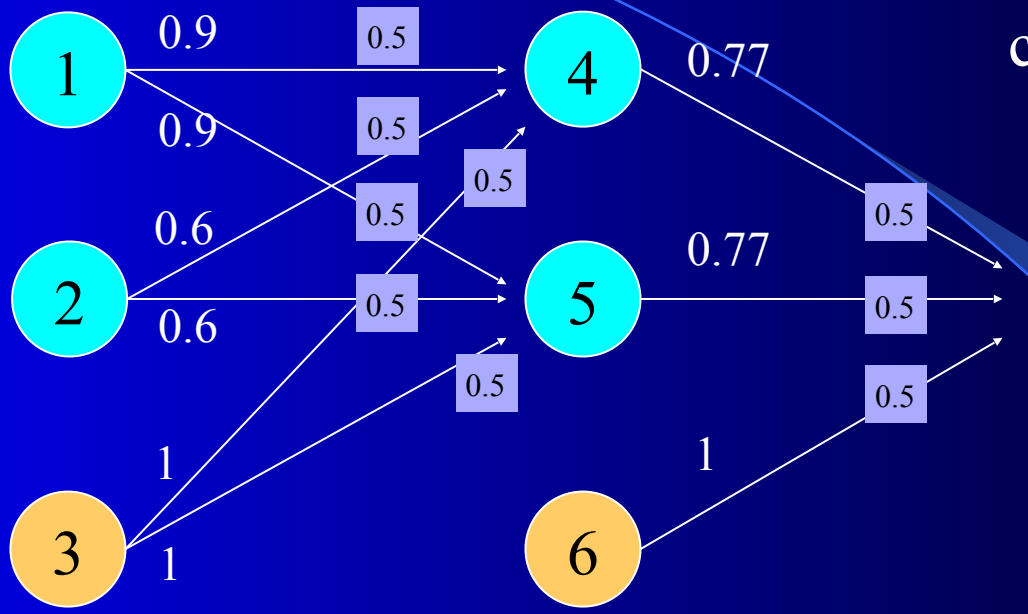
$net_5 = 1.25$

$z_4 = 1/(1 + e^{-1.25}) = .777$

$z_5 = .777$

$net_7 = .777 * .5 + .777 * .5 + 1 * .5 = 1.277$



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$net_5 = 1.25$

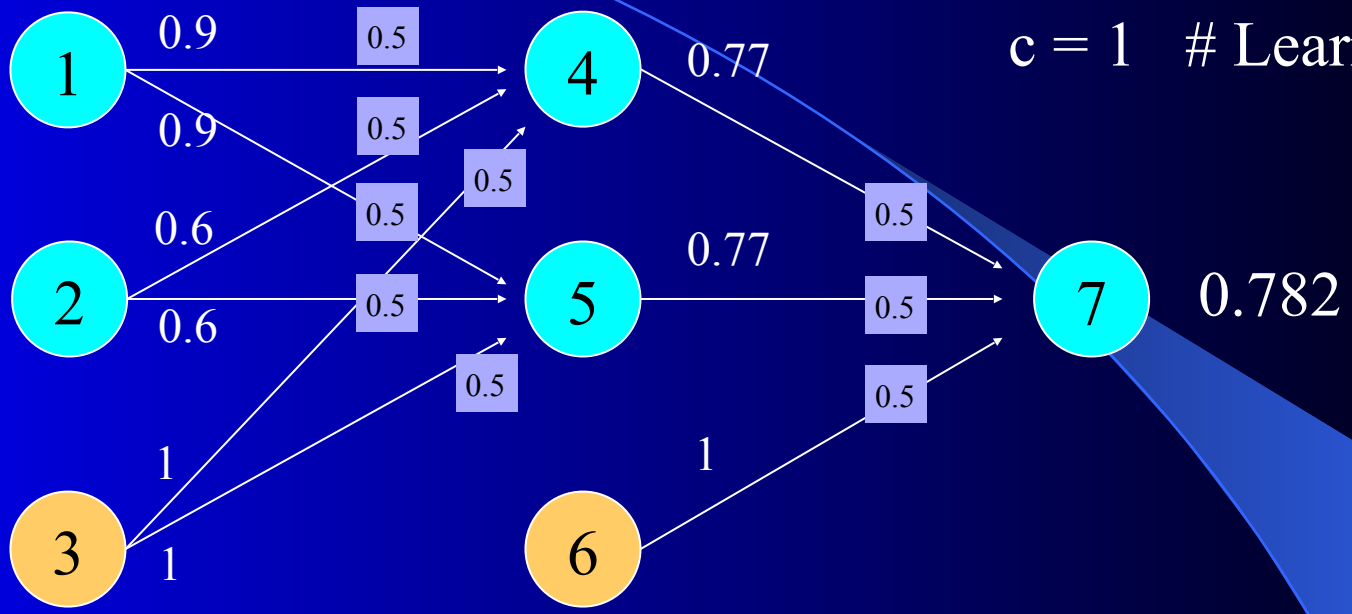
$z_4 = 1/(1 + e^{-1.25}) = .777$

$z_5 = .777$

$net_7 = .777 * .5 + .777 * .5 + 1 * .5 = 1.277$

$z_7 = 1/(1 + e^{-1.277}) = .782$

Calculate δ_j



Output node – only one

$$\delta_j = (t_j - z_j) \cdot z_j \cdot (1 - z_j)$$

$\delta_7 = (0 - .782) * .782 * (1 - .782) = -.133$

Hidden nodes – only have node 7 following

$$\delta_i = \left(\sum_{k \in follows(i)} \delta_k w_{ik} \right) \cdot z_i \cdot (1 - z_i)$$

$\delta_4 = (-.133 * .5) * .777 * (1 - .777) = -.0115$

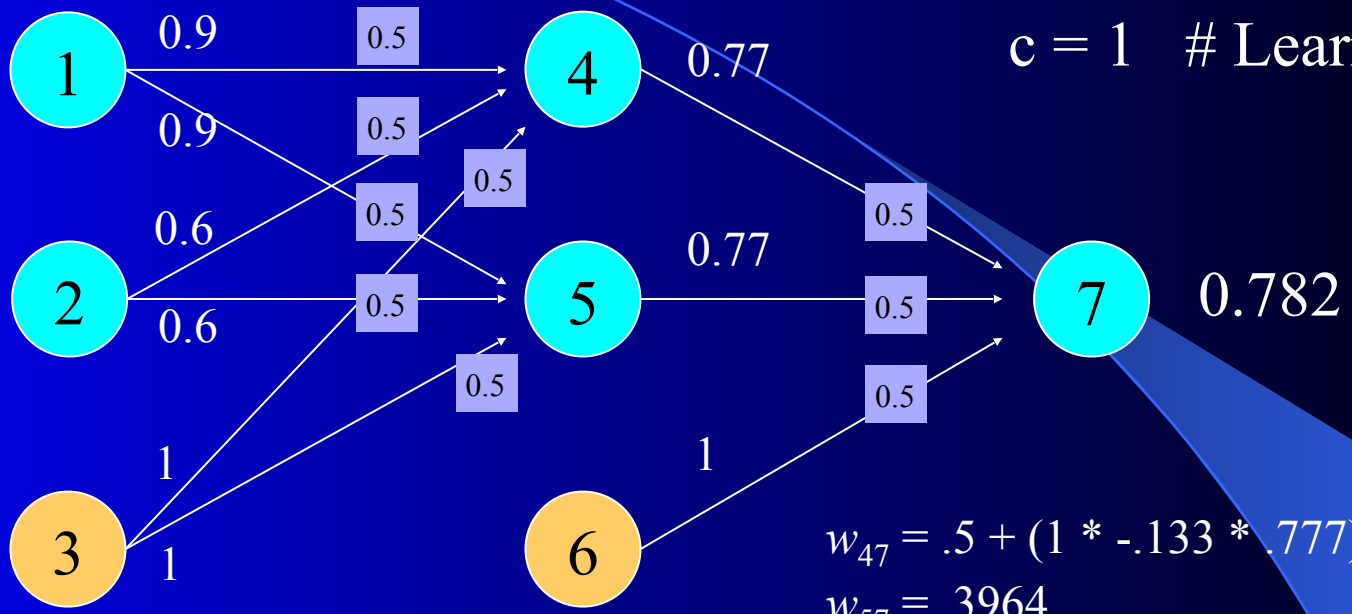
$\delta_5 = -.0115$

Calculate new weights

0.5 Weights

t = 0

c = 1 # Learning Rate



$$w_{ij} = w_{ij} + c \cdot \delta_j \cdot z_i$$

$w_{47} = .5 + (1 * -.133 * .777) = .3964$

$w_{57} = .3964$

$w_{67} = .5 + (1 * -.133 * 1) = .3667$

$w_{14} = .5 + (1 * -.0115 * .9) = .4896$

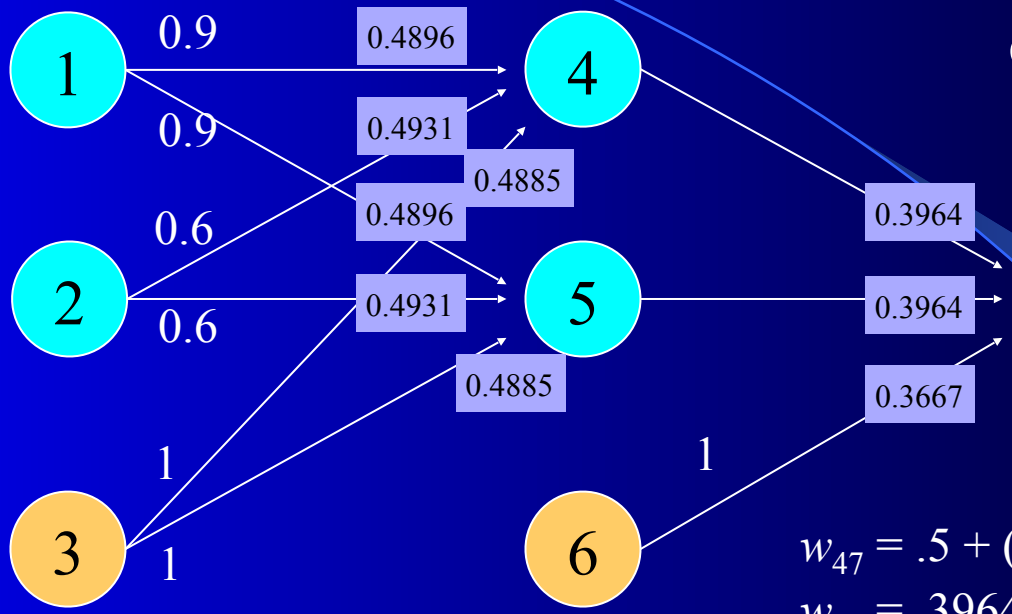
$w_{15} = .4896$

$w_{24} = .5 + (1 * -.0115 * .6) = .4931$

$w_{25} = .4931$

$w_{34} = .5 + (1 * -.0115 * 1) = .4885$

$w_{35} = .4885$



0.5 Weights

t = 0

c = 1 # Learning Rate

$$w_{ij} = w_{ij} + c \cdot \delta_j \cdot z_i$$

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$w_{34} = .5 + (1 * -.0115 * 1) = .4885$

$w_{35} = .4885$

Backpropagation Learning Example

$net_4 = .9 * .5 + .6 * .5 + 1 * .5 = 1.25$
$net_5 = 1.25$

$z_4 = 1/(1 + e^{-1.25}) = .777$
$z_5 = .777$

$net_7 = .777 * .5 + .777 * .5 + 1 * .5 = 1.277$

$z_7 = 1/(1 + e^{-1.277}) = .782$

$\delta_7 = (0 - .782) * .782 * (1 - .782) = -.133$
$\delta_4 = (-.133 * .5) * .777 * (1 - .777) = -.0115$
$\delta_5 = -.0115$

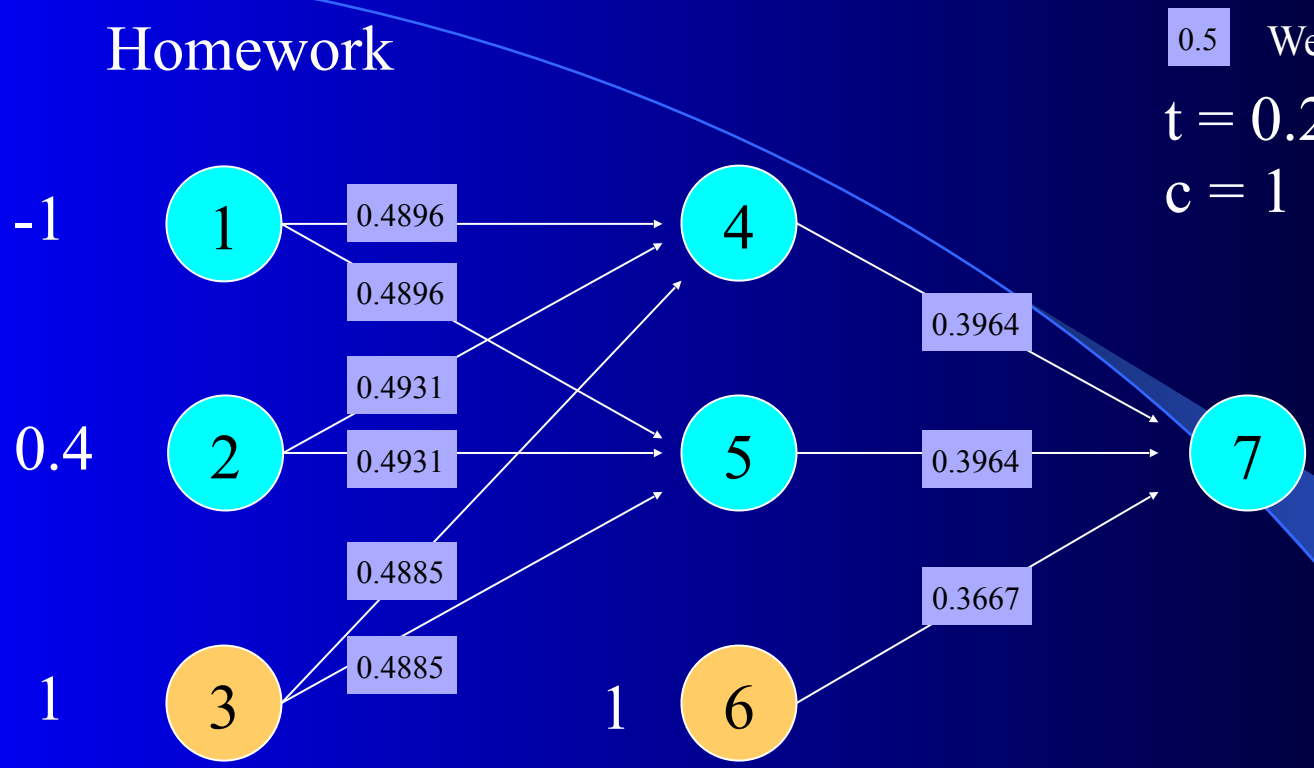
$w_{47} = .5 + (1 * -.133 * .777) = .3964$
$w_{57} = .3964$
$w_{67} = .5 + (1 * -.133 * 1) = .3667$

$w_{14} = .5 + (1 * -. 0115 * .9) = . 4896$
$w_{15} = .4896$

$w_{24} = .5 + (1 * -. 0115 * .6) = . 4931$
$w_{25} = .4931$

$w_{34} = .5 + (1 * -. 0115 * 1) = .4885$
$w_{35} = .4885$

Homework



Evaluate the network using the new weights on the new input

Using those values, back propagate the error and calculate new weights for the network

Backprop Homework

- For your homework, update the weights for a second instance -1 .4 ==> .2. Continue using the updated weights shown on the previous slide. Show your work like we did on the previous slide.

- Then go to the link below: Neural Network Playground and play around with the BP simulation. Try different training sets, layers, inputs, etc. and get a feel for what the nodes are doing. **You do not have to hand anything in for this part.**

- http://playground.tensorflow.org/

MLP/Backpropagation Summary

- Excellent empirical results
- Scaling – The pleasant surprise
  - Local minima very rare as problem and network complexity increase
- Hyper-parameters usually handled by trial and error
- Many variants
  - Adaptive Parameters, ontogenic (growing and pruning) learning algorithms
  - Many different architectures
    - Recurrent networks
    - Deep networks
  - An active research area