Data Mining and Machine Learning

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Introduction to Artificial Neural Networks

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Objectives

- Introduce Artificial Neural Networks (ANNs)
- Feed-forward ANNs – **Multi-Layer Perceptrons** (MLPs)
- Basic MLP calculations
- Geometric interpretation of MLPs

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Artificial Neural Networks

- (Artificial) Neural Networks (NNs) offer another approach to data analysis
- Popularised in 1980s, resurgence in 2000s
- "Machine learning" (or most recently "AI") often synonymous with the use of NNs
- Inspiration for the basic elements of a NN (artificial neuron) comes from biology, but analogy stops there
- ANNs are just a computational device for processing patterns – not "artificial brains"

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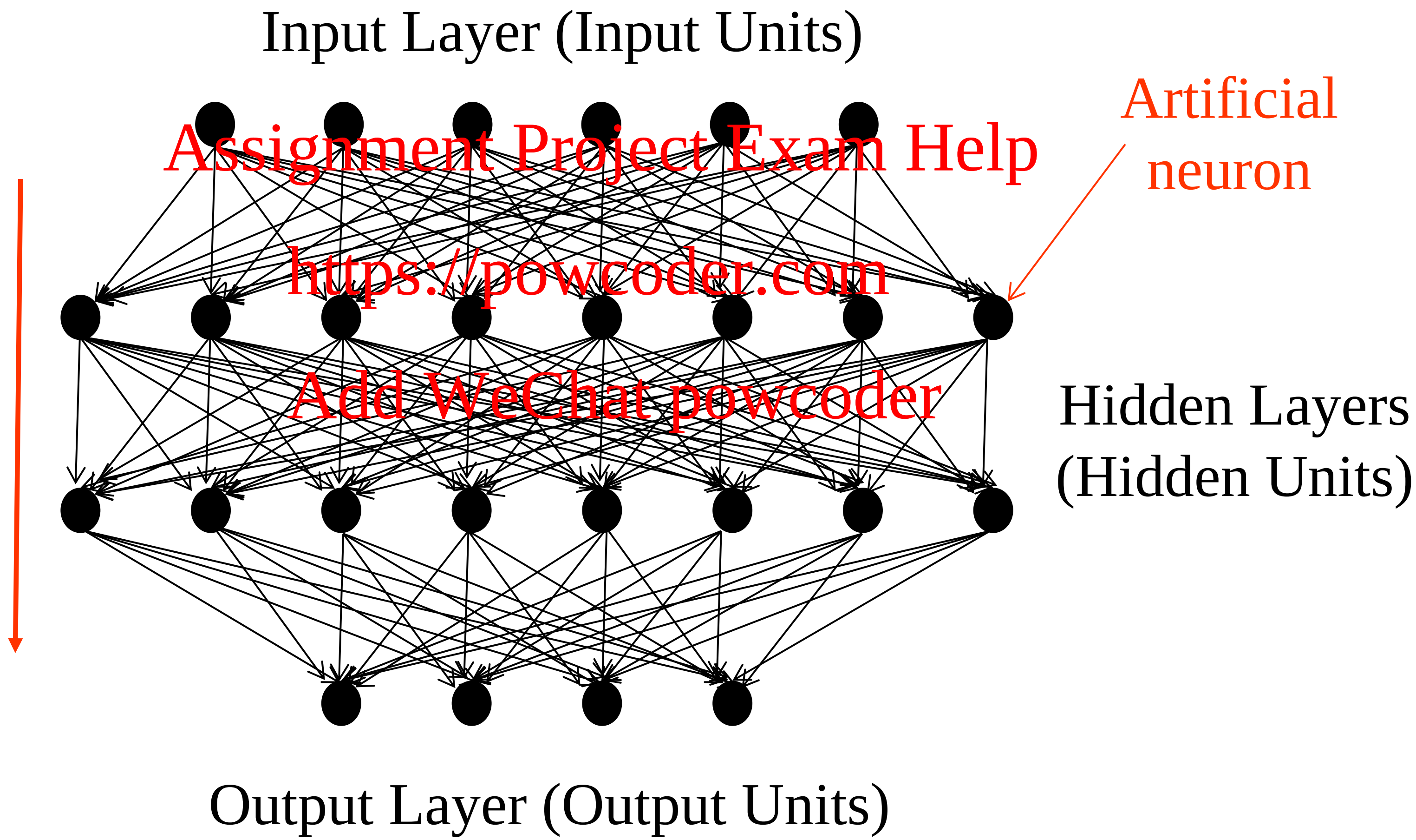
Feed-forward Neural Networks

Multi-Layer Perceptron - Feed-Forward Neural Network



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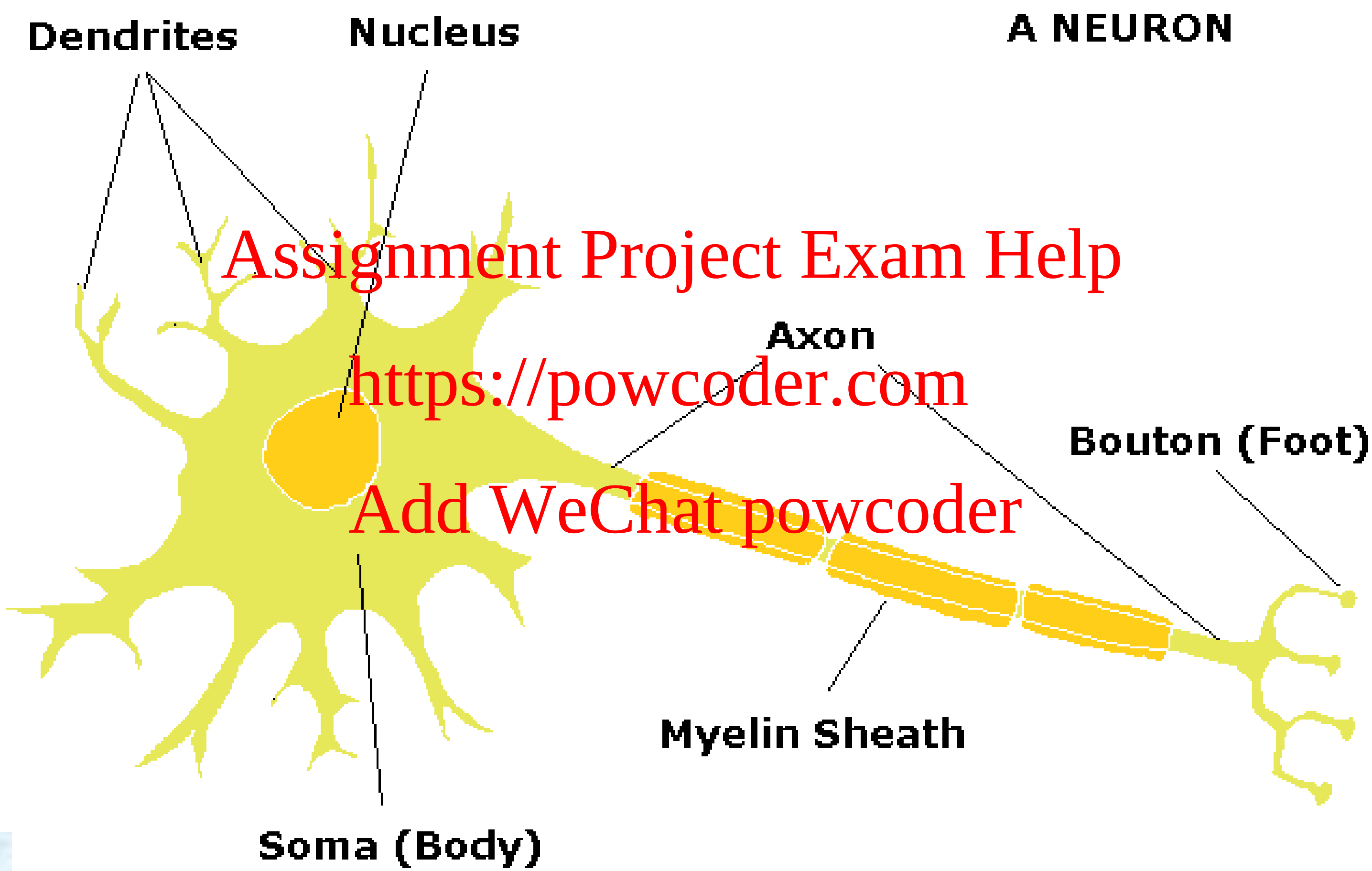
A simple model of a neuron



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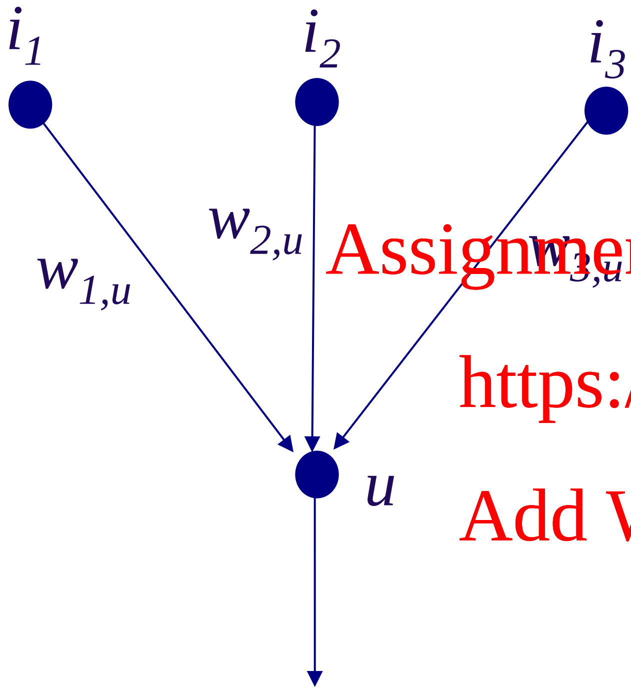
A Simple Artificial Neuron



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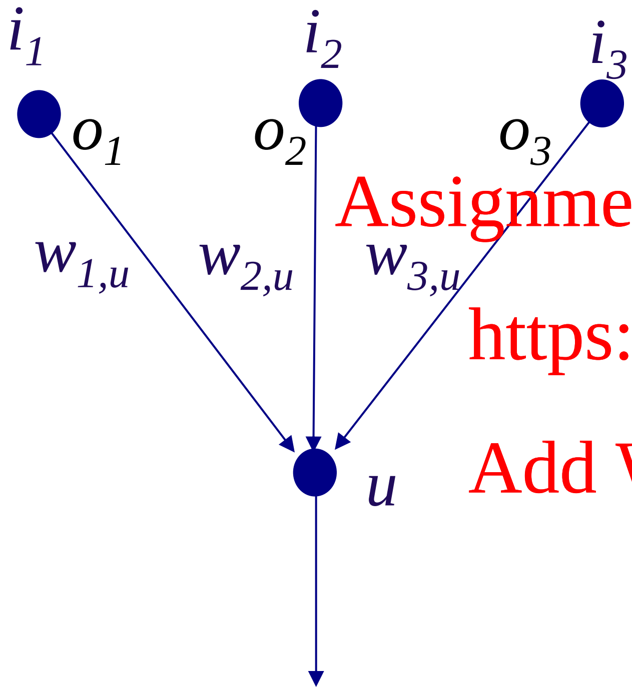
- Basic idea –
  - if the input i_u to unit u is big enough, the neurone 'fires'
  - Otherwise nothing happens
- How do we calculate the input to u?

Artificial Neurone (2)



- Suppose the inputs to units 1, 2 and 3 are i_1, i_2 and i_3 and these are also the outputs o_1, o_2 and o_3
- Then the input to u is:

$$i_u = o_1 w_{1,u} + o_2 w_{2,u} + o_3 w_{3,u}$$

- In general, for an artificial neuron u that receives input from N units, the input to unit u is:

$$i_u = \sum_{n=1}^{N} o_n w_{n,u}$$

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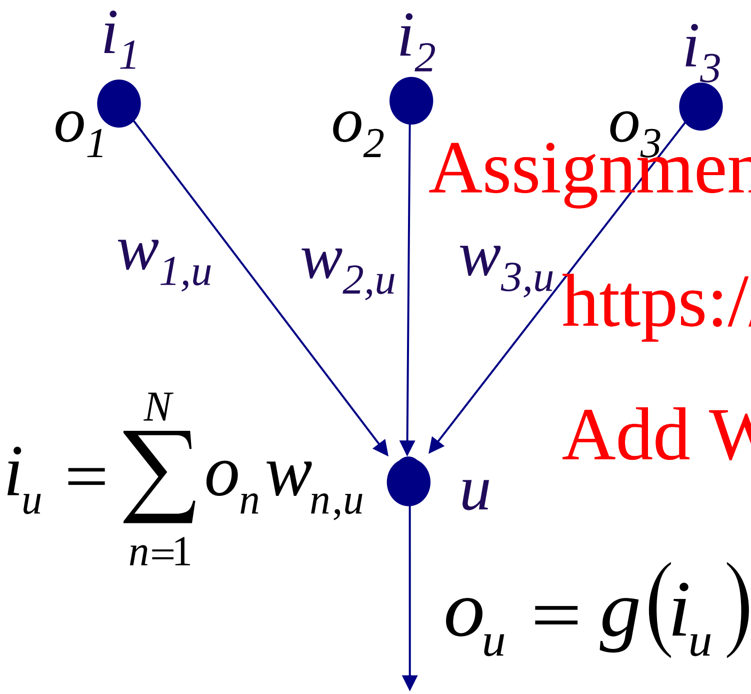
The sigmoid activation function



- The <u>activation function</u> defines the output of a neuron - whether the neuron should "fire"
- A typical activation function is the sigmoid function g:

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

- The output of u is then:

$$o_u = g(i_u)$$

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Activation functions

- Linear activation function (output equals input):

$$g(x) = x$$

- Sigmoid activation function:

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

- The sigmoid is a 'soft' threshold function

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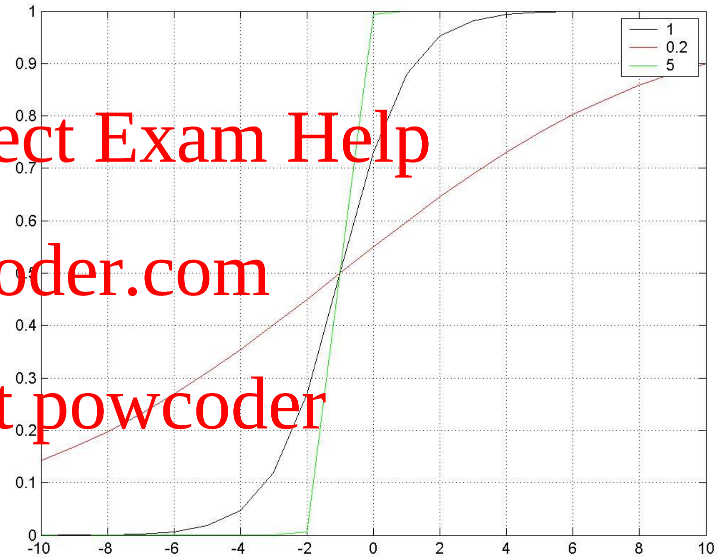
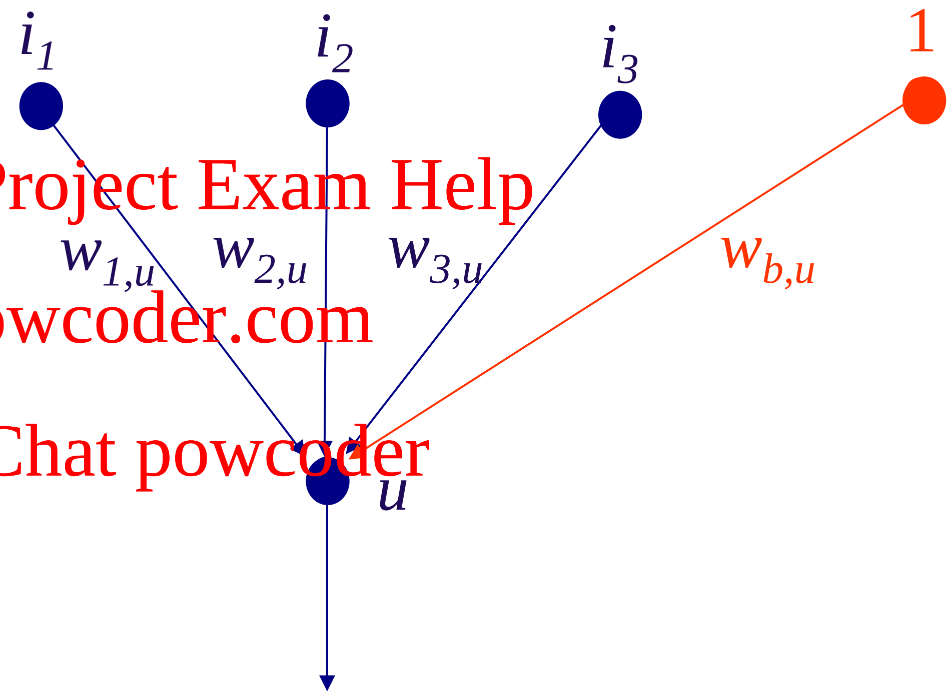


Sigmoid activation function

The 'bias'

- As described, the neuron will 'fire' only if its input is greater than 0
- We can change the value of the point of firing by introducing a <u>bias</u>
- This is an additional input unit whose input is fixed at 1



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How the bias works…

- According to the sigmoid activation function, the artificial neuron *u* ‘fires’ if the input to *u* is greater than or equal to 0

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- i.e: $i_u = o_1 w_{1,u} + o_2 w_{2,u} + o_3 w_{3,u} + w_{b,u} \geq 0$

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- But this happens only if

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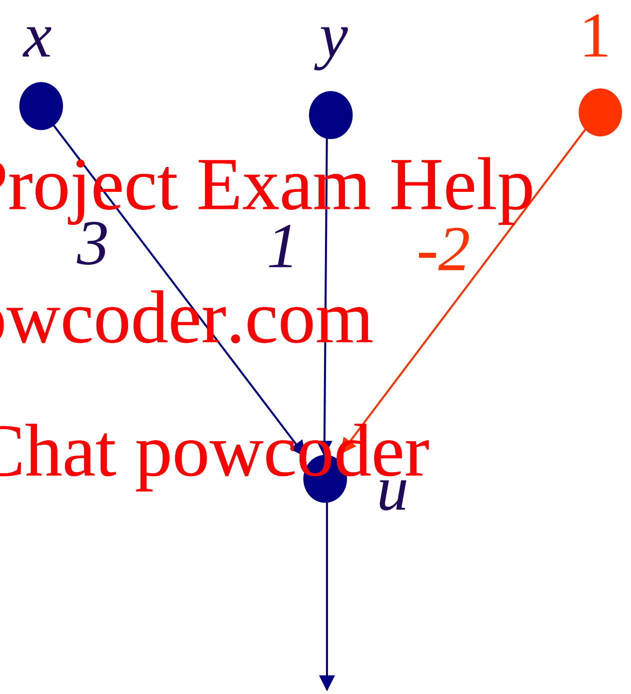
$$i_1 w_{1,u} + i_2 w_{2,u} + i_3 w_{3,u} \geq -w_{b,u}$$

Example (2D)

- Suppose u has a sigmoid activation function. Then, for these values of weight, u will ‘fire’ if:

$$i_u = 3x + y - 2 \geq 0$$

i.e. $y \geq -3x + 2$



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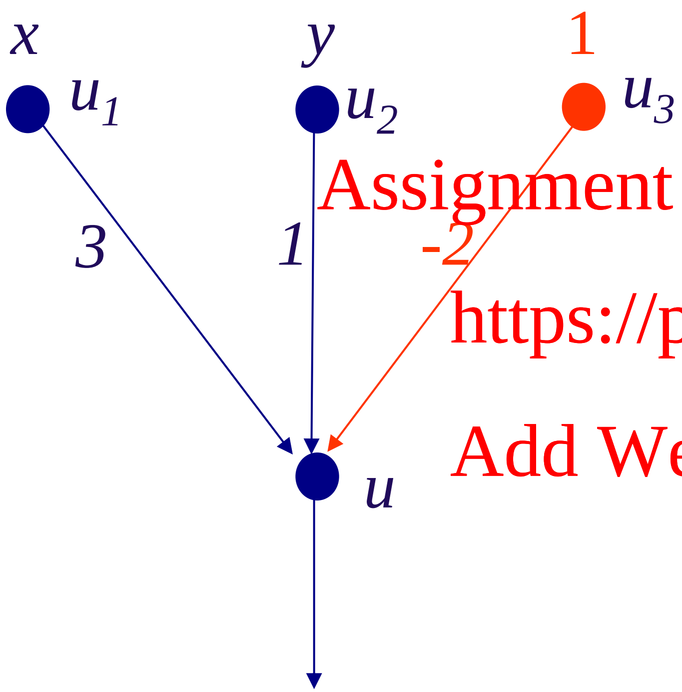
Example (continued)



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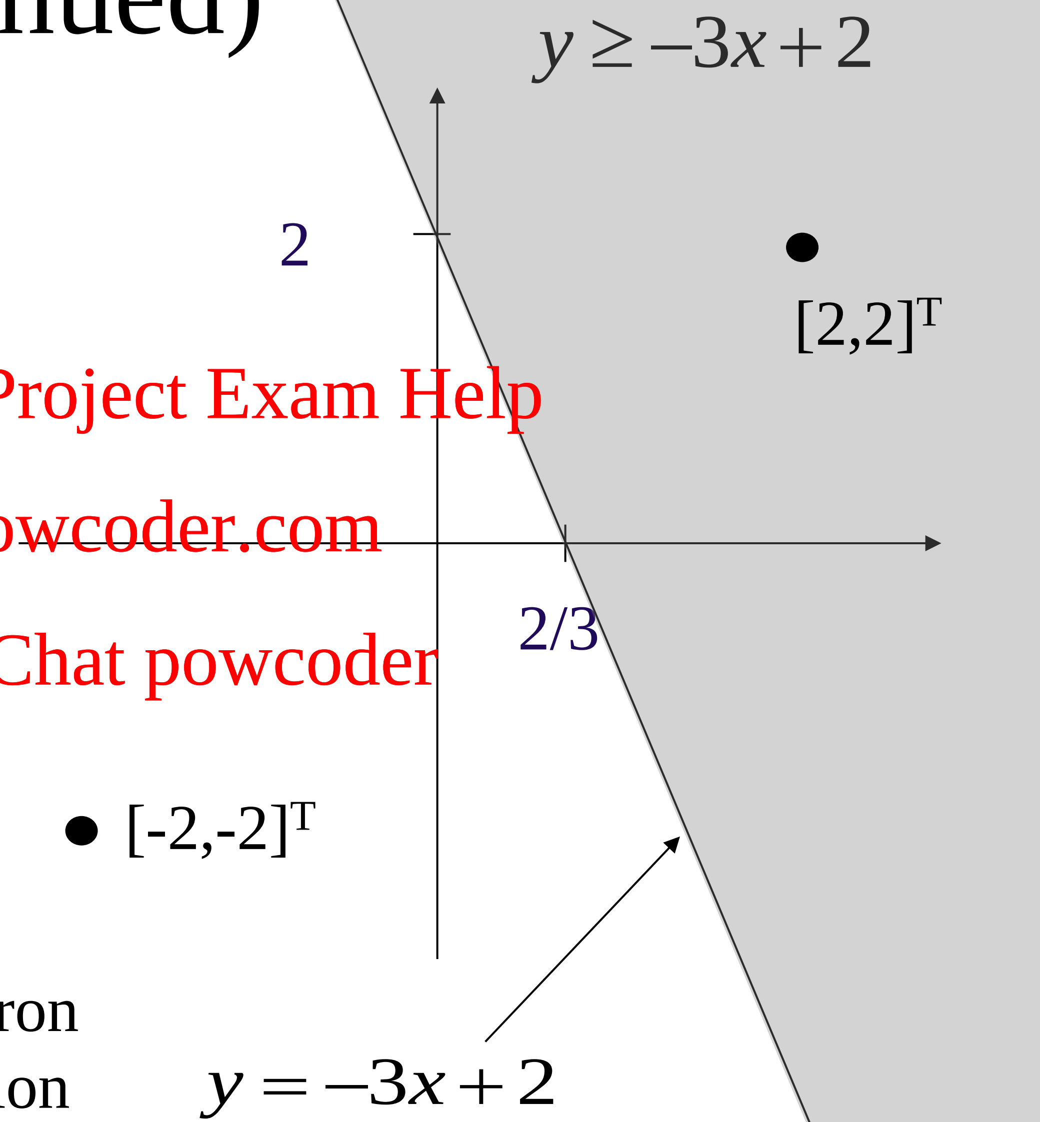

A single artificial neuron defines a linear decision boundary

Example (continued)

- Assume
  - Linear activation functions for units u_1, u_2 and u_3
  - Sigmoid activation function for u
- <u>Case1</u>: input to u_1 is 2 and input to u_2 is 2, then:
  - Input i_u to u is $2 \times 3 + 2 \times 1 + 1 \times (-2) = 6$
  - Hence output o_u from u is $g(6) = 0.998$
- <u>Case</u> 2: input to u_1 is -2 and input to u_2 is -2, then:
  - Input i_u to u is $-2 \times 3 + -2 \times 1 + 1 \times (-2) = -10$
  - Hence output o_u from u is $g(-10) = 4.54 \times 10^{-5} \approx 0$

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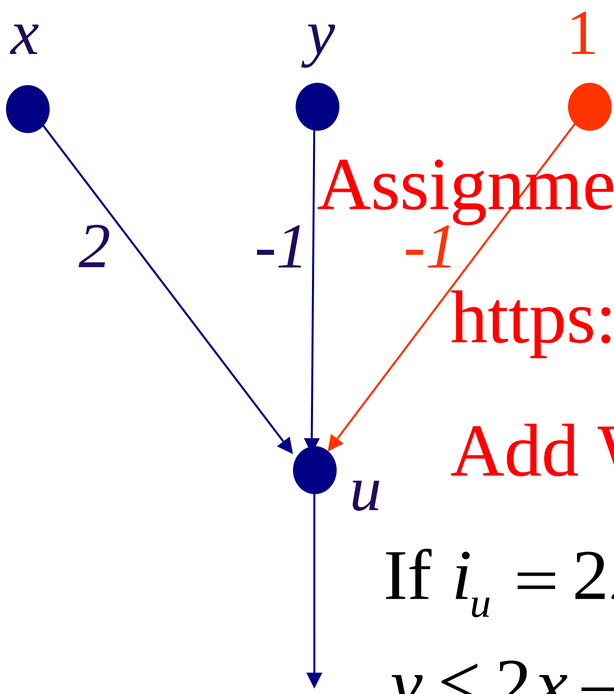
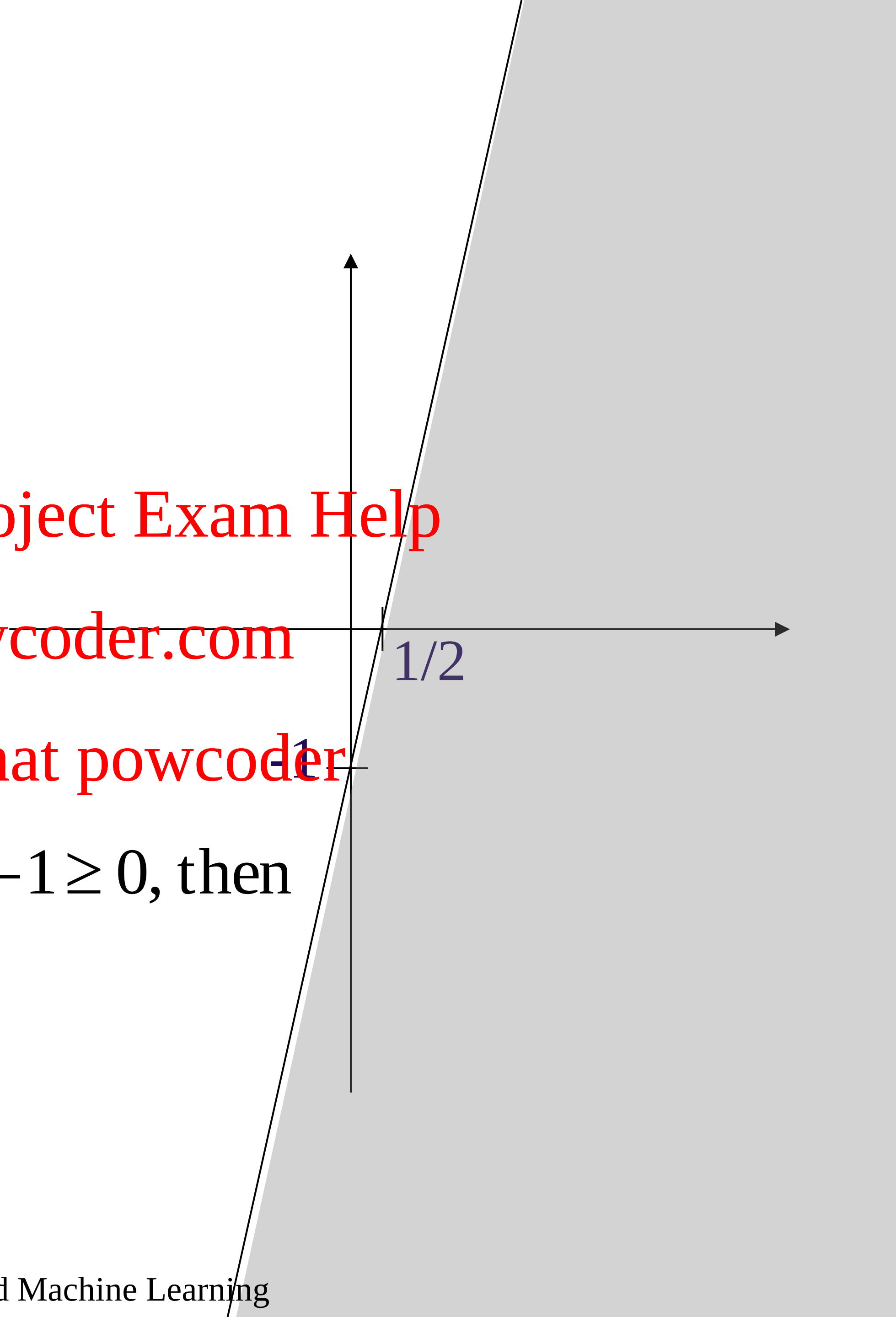
Example 2





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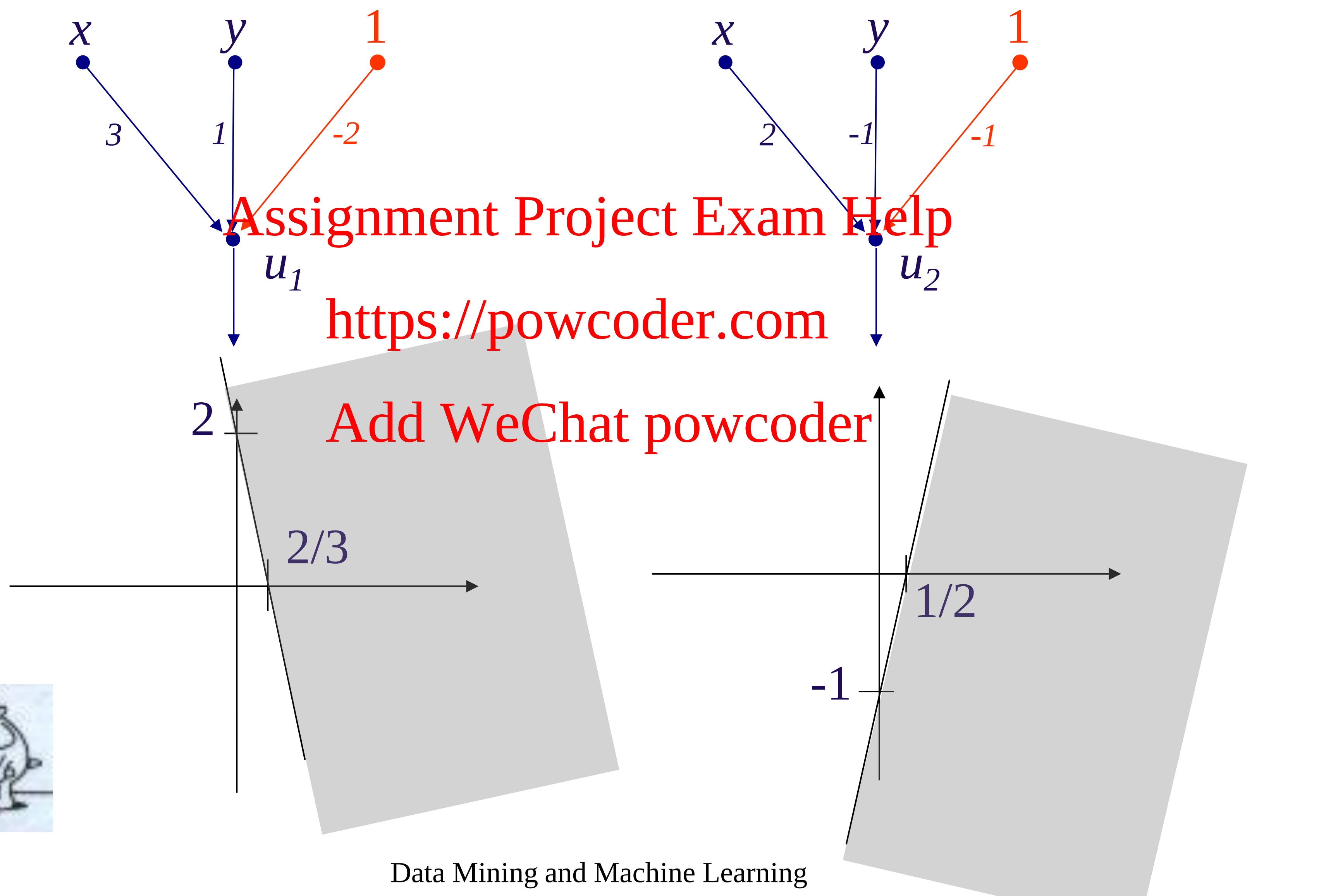
If $i_u = 2x - y - 1 \geq 0$, then

$y \leq 2x - 1$

Combining 2 Artificial Neurons



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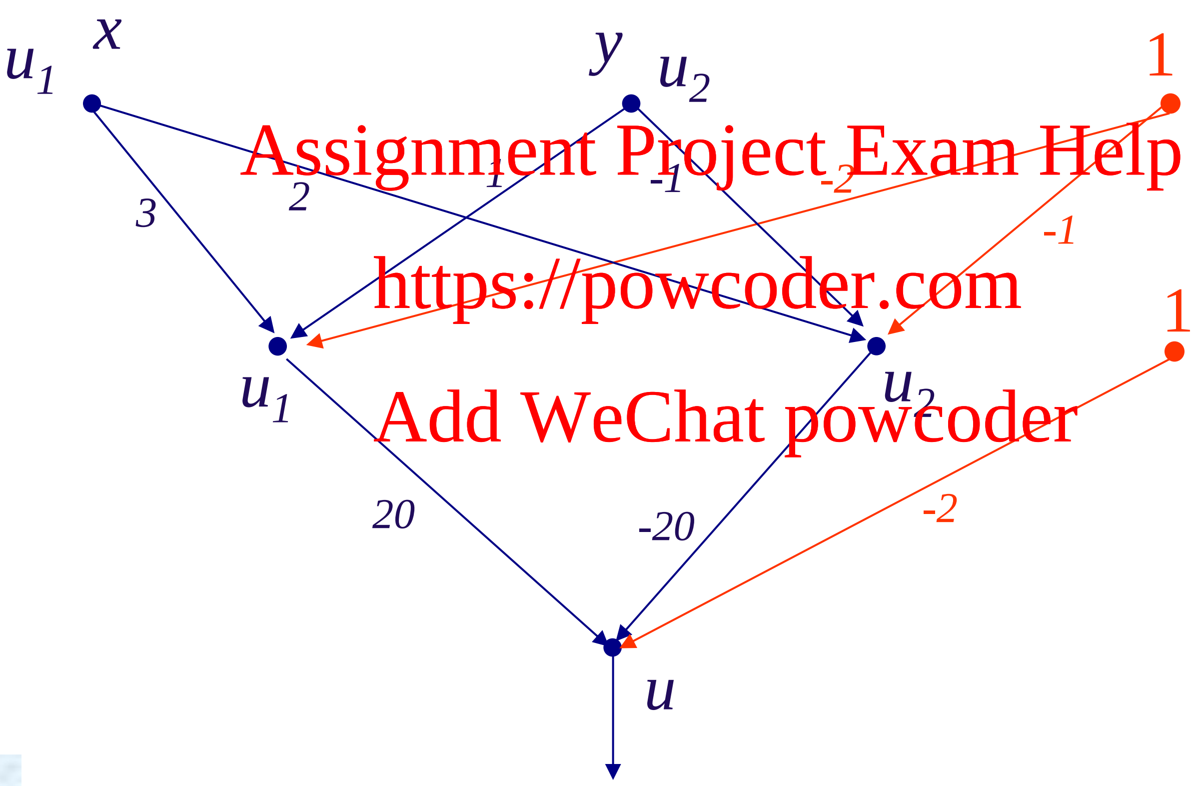
Combining neurons – artificial neural networks



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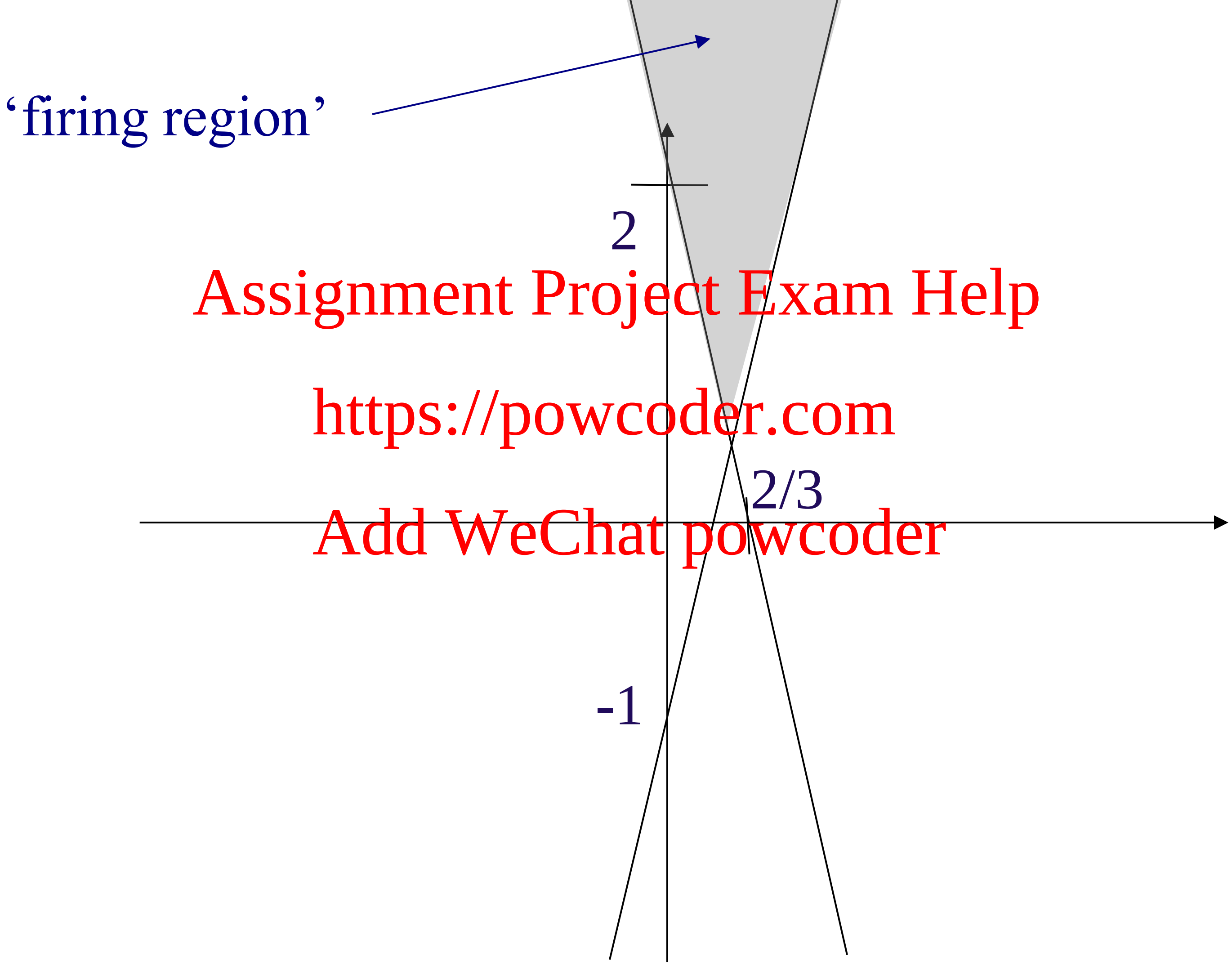
Combining neurones



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Combining neurons

- Input to u_1 is $3x + y - 2$
- Input to u_2 is $2x - y - 1$
- When $x = 3$, $y = 0$
  - Input i_{u1} to u_1 is 7; input i_{u2} to u_2 is 5
  - Output o_{u1} from u_1 is 1, output o_{u2} from u_2 is 0.993
  - Input i_u to u is $1 \times 20 + 0.993 \times (-20) - 2 = -1.88$
  - Output o_u from u is $g(-1.88) = 0.13$

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Outputs

i_1	i_2	o_u
3	0	0.13
0.5	2	1.00
0.5	-2	0.00
-1	0	0.06

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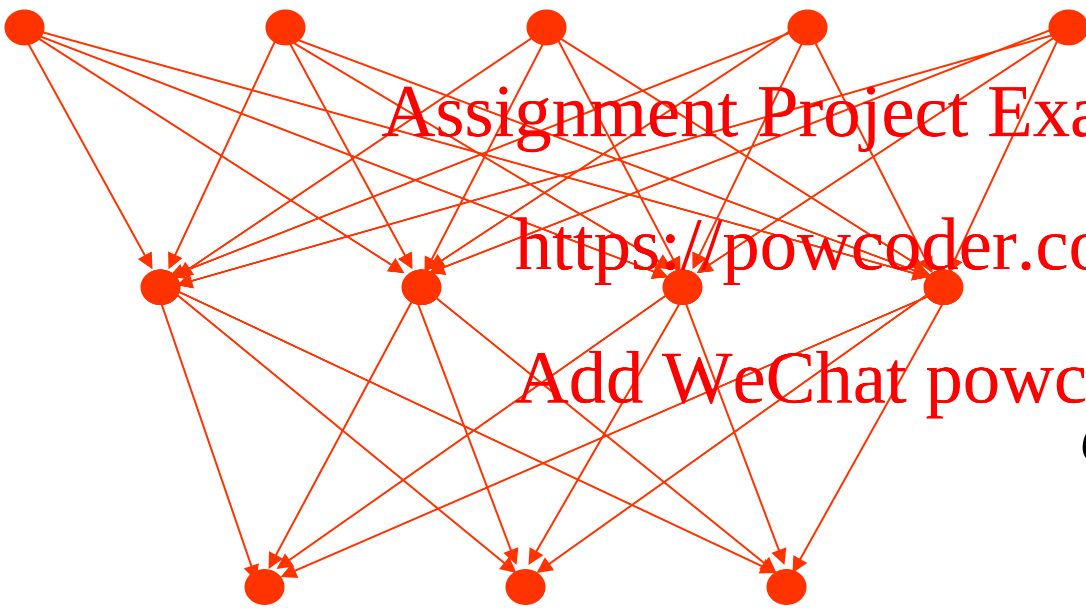
Single hidden layer Multi-Layer Perceptron (MLP)



I units in Input layer

$H \times I$ weight matrix $\boldsymbol{W^1}$

H units in Hidden layer

$O \times H$ weight matrix $\boldsymbol{W^2}$

O units in Output layer

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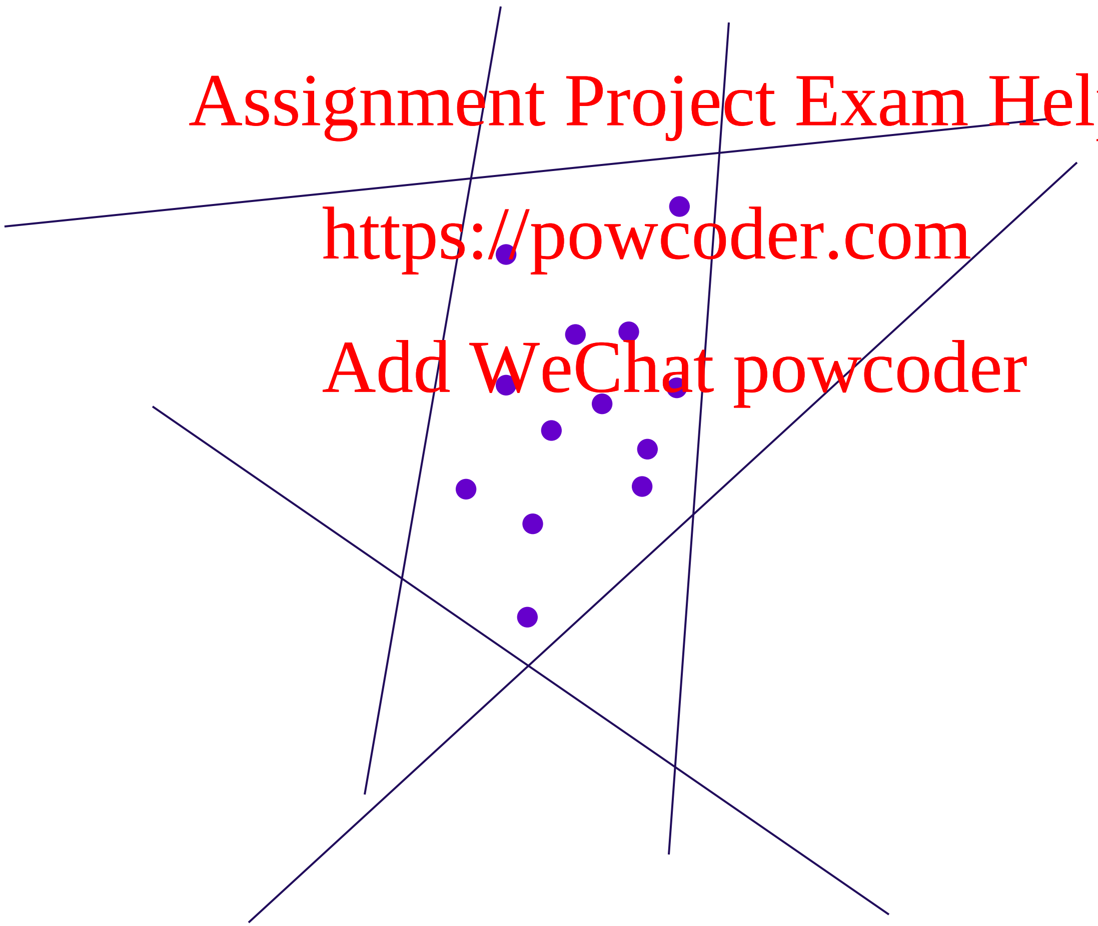
Single hidden layer MLP

- Can characterize arbitrary convex regions
- Defines the region using linear decision boundaries



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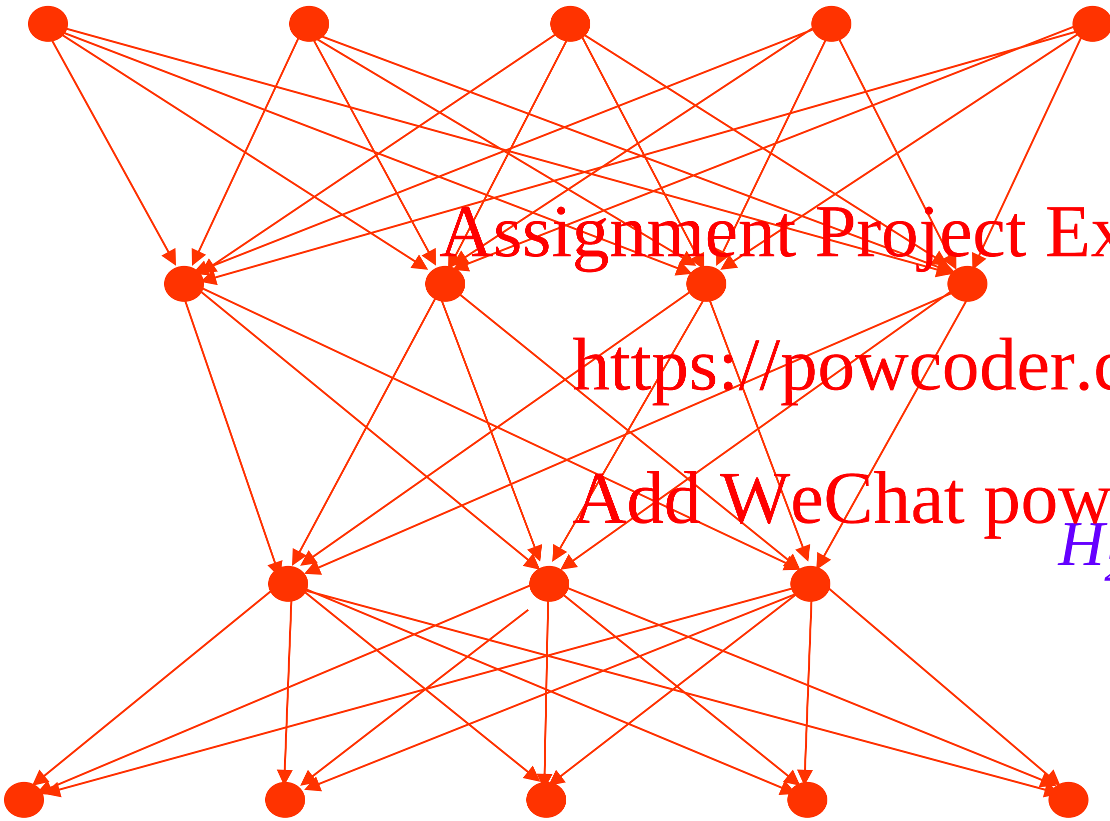
Two hidden layer MLP



I units in Input layer

$H_1 \times I$ weight matrix $\boldsymbol{W^1}$

H_1 units in first hidden layer

$H_2 \times H_1$ weight matrix $\boldsymbol{W^2}$

H_2 units in second hidden layer

$O \times H_2$ weight matrix $\boldsymbol{W^3}$

O units in Output layer

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Two hidden layer MLP

- An MLP with two hidden layers can characterize arbitrary shapes
- First hidden layer characterises convex regions
- Second hidden layer combines these convex regions
- In theory, there is no advantage in having more than two hidden layers
- In practice multiple hidden layer “deep” neural networks give best performance (e.g. Speech recognition)

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Formal definition: MLP with a single hidden layer

- A single hidden layer MLP consists of:
  1. A set of I input units, and for each input unit i an activation function g_i (typically linear)
  2. A set of H hidden units, and for each hidden unit h an activation function g_h (typically sigmoid)
  3. A set of O output units, and for each output unit o an activation function g_o
  4. An H x I weight matrix W^1, which maps the outputs of the input units to the inputs of the hidden units
  5. An O x H weight matrix W^2, which maps the outputs of the hidden units to the inputs of the output units

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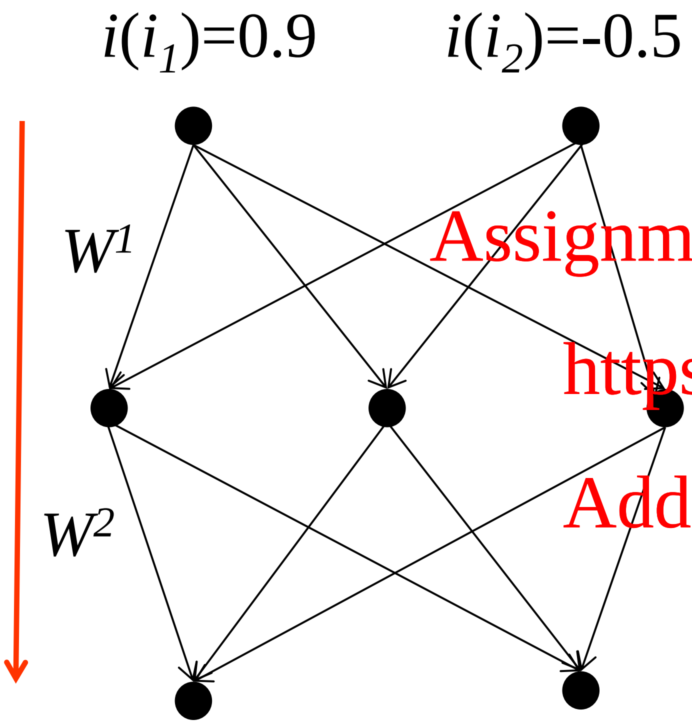
Example



- 2 unit input layer, linear activation (I = 2)
- Single 3 unit hidden layer, sigmoid activation (H = 3)
- 2 unit output layer, linear activation (O = 2)
- A 3 x 2 weight matrix W^1 between input and hidden layer
- A 2 x 3 weight matrix W^2 between hidden and output layer

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Example continued

$$W^1 = \begin{bmatrix} 2.6 & -1.7 \\ 0.2 & 1.0 \\ -4.0 & 2.5 \end{bmatrix}, W^2 = \begin{bmatrix} 1.0 & -0.5 & 1.0 \\ 0.5 & 0.6 & -1.0 \end{bmatrix}$$

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$$\text{Input} = \begin{bmatrix} 0.9 \\ -0.5 \end{bmatrix}$$

$$\text{Output from first layer} = \begin{bmatrix} 0.9 \\ -0.5 \end{bmatrix} \text{(linear activation)}$$

Example (continued)

Inputs to hidden layer:

$$i(h_1) = w_{11}^1 o_1 + w_{12}^1 o_2 = 2.6 \times 0.9 + (-1.7) \times \left(-0.5\right) = 2.34 + 0.85 = 3.19,$$

$$i\left(h_2\right) = w_{21}^1 o_1 + w_{22}^1 o_2 = 0.2 \times 0.9 + 1.0 \times (-0.5) = 0.18 - 0.5 = -0.32,$$

$$i\left(h_3\right) = w_{31}^1 o_1 + w_{32}^1 o_2 = (-4.0) \times 0.9 + 2.5 \times (-0.5) = -3.6 - 1.25 = -4.85$$

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In matrix notation:

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$$i\left(h\right) = W^1 o$$

Outputs from hidden layer:

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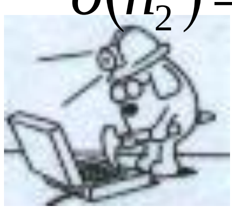
$$o(h_1) = \frac{1}{1+e^{-3.19}} = 0.96,$$

$$o\left(h_2\right) = \frac{1}{1+e^{0.32}} = 0.42, \; o\left(h_3\right) = \frac{1}{1+e^{4.85}} = 0.008.$$



Example (continued)

Inputs to the output layer :

$$i(o_1) = w_{11}^2 \times o(h_1) + w_{12}^2 \times o(h_2) + w_{13}^2 \times o(h_3)$$

$$i(o_1) = 1 \times 0.96 + (-0.5) \times 0.42 + 1 \times 0.008 = 0.96 - 0.21 + 0.008 = 0.758.$$

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$$i(o_2) = w_{21}^2 \times o(h_1) + w_{22}^2 \times o(h_2) + w_{23}^2 \times o(h_3)$$

$$i(o_2) = 0.5 \times 0.96 + 0.6 \times 0.42 - 1 \times 0.008 = 0.48 + 0.254 - 0.008 = 0.742.$$

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In matrix notation :

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$$i(o) = W^2 o(h)$$

Linear output unit activation :

$$o(o_1) = 0.758, \; o(o_2) = 0.742.$$

Summary

- Introduction to neural networks
- Definition of an ‘artificial neurone’
- Activation functions – linear and sigmoid
- Linear boundary defined by a single neurone
- Convex region defined by a one-level MLP
- Two-level MLPs
- Forward propagation in an MLP (calculation)

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