Backpropagation

COMP 4630 | Winter 2025

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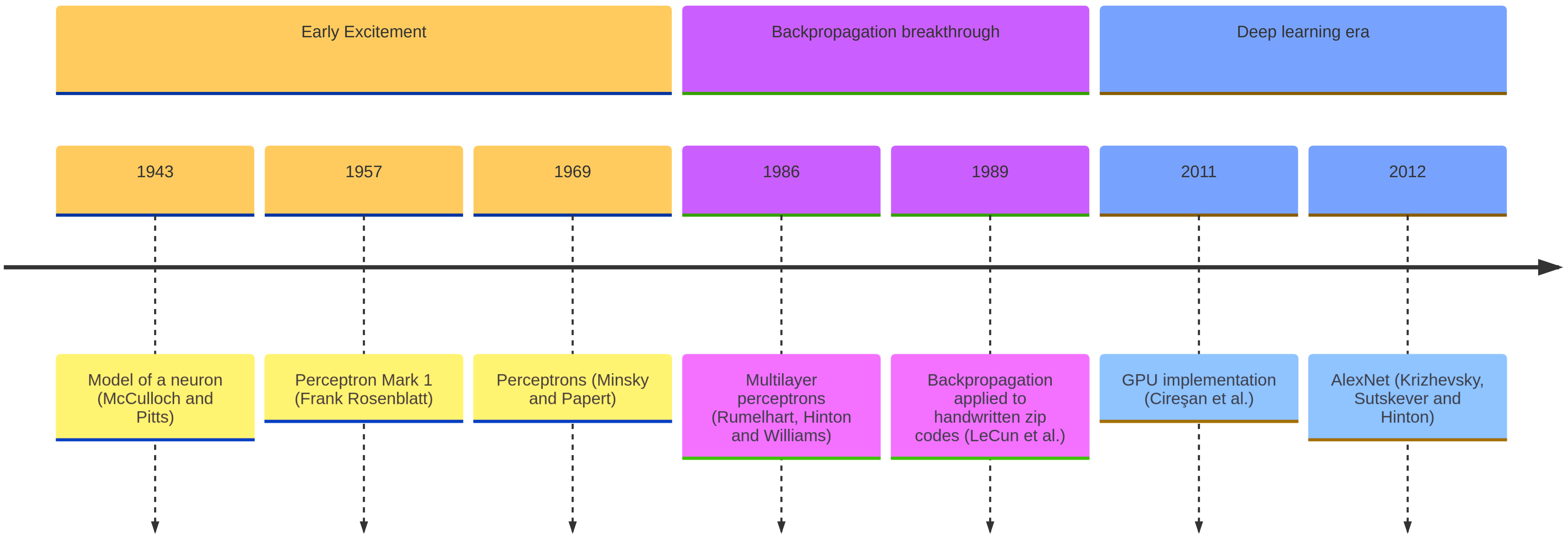
Overview

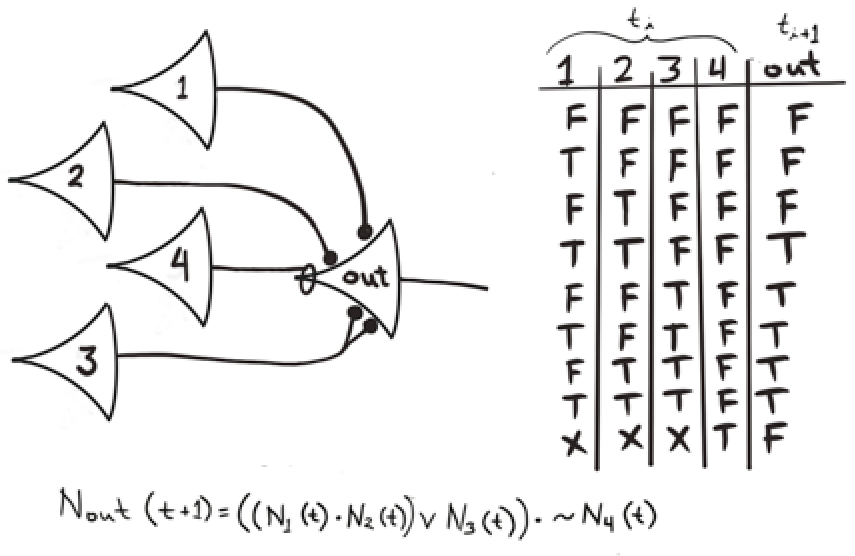
- A brief review of the history of neural networks
- Neurons, perceptrons, and multilayer perceptrons
- Backpropagation
- References and suggested reading:
    - Scikit-learn book: Chapter 10, introduction to artificial neural networks
    - Deep Learning Book: Chapter 6, deep feedforward networks

The rise and fall of neural networks



In between each era of excitement and advancement there was an "AI winter"

Model of a neuron

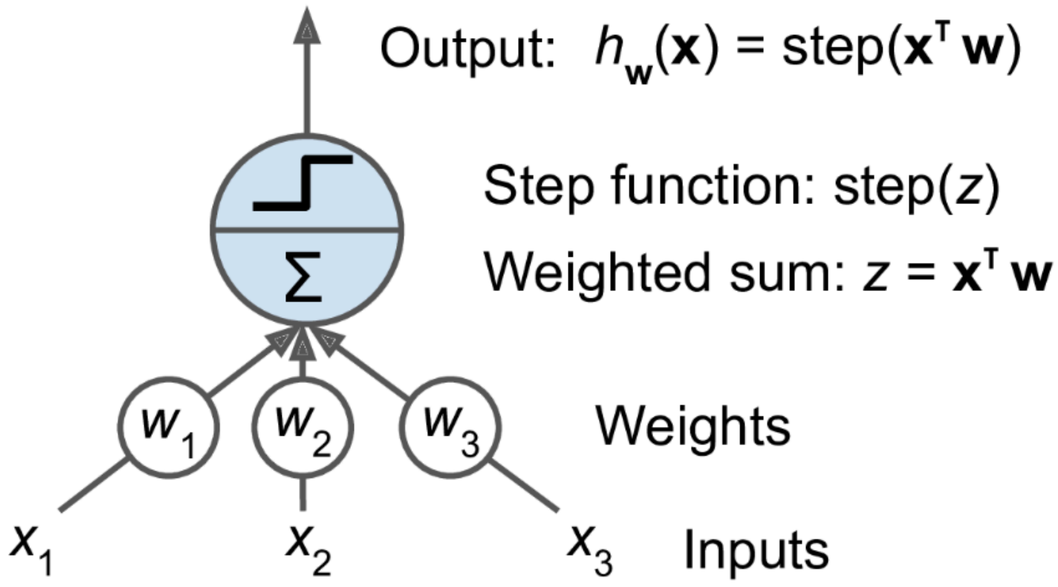


- McCulloch and Pitts (1943)
- Neuron as a logic gate with time delay
- "Activates" when the sum of inputs exceeds a threshold
- Non-invertible (forward propagation only)

Further reading: Original Paper (rather dense math) or an Accessible webpage

Threshold Linear Units (TLUs)

- Linear I/O instead of binary
- Rosenblatt (1957) combined multiple TLUs in a single layer
- Physical machine: the Mark I Perceptron, designed for image recognition
- Criticized by Minsky and Papert (1969) for its inability to solve the XOR problem - first AI winter



A single threshold logic unit (TLU)

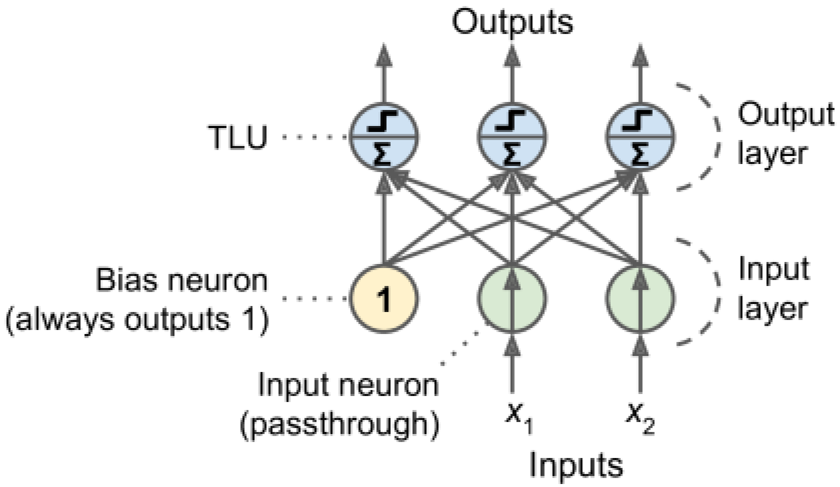
Image source: Scikit-learn book

Training a perceptron

- Hebb's rule: "neurons that fire together, wire together"

  $$w_{ij}^{(updated)} = w_{ij} + \eta(y_j - \hat{y}_j)x_i$$

  where i = input, j = output
- Fed one instance at a time,
- Guaranteed to converge if inputs are **linearly separable**
- 🧮 Simple example: AND gate



A perceptron with two inputs and three outputs

Image source: Scikit-learn book

Multilayer perceptrons (MLPs)

- If a perceptron can't even solve XOR, how can it do higher order logic?
- Consider that XOR can be rewritten as:

```
A xor B = (A and !B) or (!A and B)
```

- A perceptron can solve `and` and `or` and `not`... so what if the input to the `or` perceptron is the output of two `and` perceptrons?

A solution to XOR

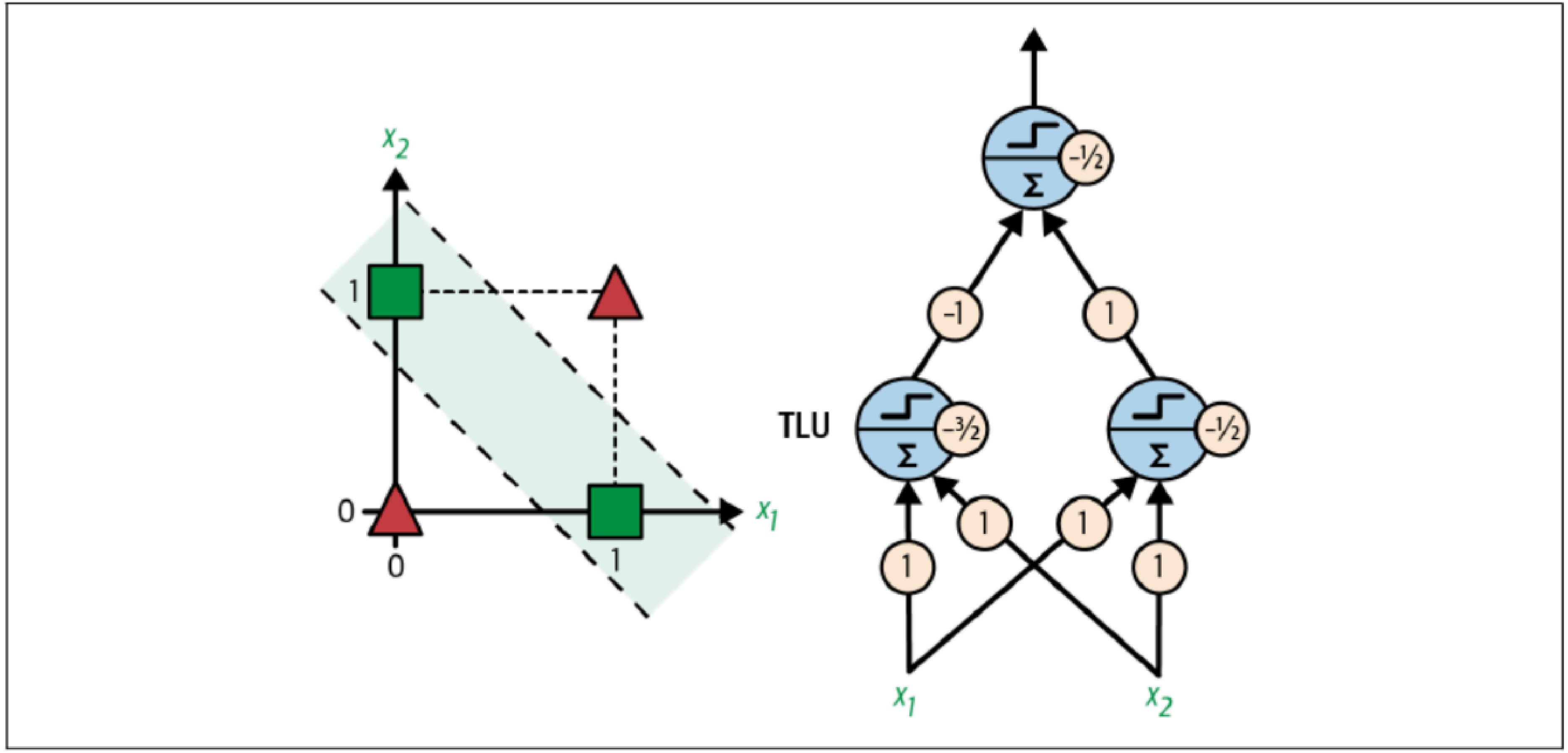


Figure 10-6. XOR classification problem and an MLP that solves it

Backpropagation

- I just gave you the weights to solve XOR, but how do we actually find them?
- Applying the perceptron learning rule no longer works, need to know how much to adjust each weight relative to the **overall output error**
- Solution presented in 1986 by Rumelhart, Hinton, and Williams
- Key insight: Good old chain rule! Plus some recursive efficiencies

Training MLPs with backpropagation

1. Initialize the weights, through some random-ish strategy
2. Perform a **forward pass** to compute the output of each neuron
3. Compute the **loss** of the output layer (e.g. MSE)
4. Calculate the **gradient of the loss** with respect to each weight
5. Update the weights using gradient descent (minibatch, stochastic, etc)
6. Repeat steps 2-5 until stopping criteria met

> *Step 4 is the "backpropagation" part*

Example: forward pass

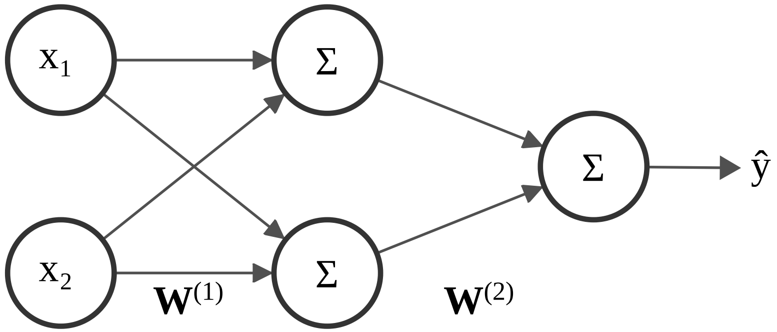
- With a linear activation function:

$$\hat{\mathbf{y}} = \mathbf{X}\mathbf{W}^{(1)}\mathbf{W}^{(2)}$$

- In summation notation for a single sample:

$$\hat{y} = \sum_{j=1}^{2} w_j^{(2)} \sum_{i=1}^{2} x_i w_{ij}^{(1)}$$

- In this case, $\hat{y} = 2.162$



$$\mathbf{x} = \begin{bmatrix} 2 & 3 \end{bmatrix}, \quad y = 1$$

and

$$\mathbf{W}^{(1)} = \begin{bmatrix} -0.78 & 0.13 \\ 0.85 & 0.23 \end{bmatrix}, \mathbf{W}^{(2)} = \begin{bmatrix} 1.8 \\ 0.40 \end{bmatrix}$$

Example: calculate error and gradient

- We never picked a loss function! Let's assume we're using MSE
- For a single sample:

$$\mathcal{L}(\mathbf{w^{(1)}}, \mathbf{w^{(2)}}) = \frac{1}{2}(\hat{y} - y)^2 = \frac{1}{2}\left(\sum_{j=1}^{2} w_j^{(2)} \sum_{i=1}^{2} x_i w_{ij}^{(1)} - y\right)^2$$

  with the $1/2$ added for convenience
- The goal is to update each weight by a small amount to minimize the loss
- Fortunately, we know how to find a small change in a function with respect to one of the variables: the partial derivative!

Recursively applying the chain rule

- Weights in the second layer (connecting hidden and output):

$$\frac{\partial \mathcal{L}}{\partial w_j^{(2)}} = \frac{\partial \mathcal{L}}{\partial \hat{y}} \frac{\partial \hat{y}}{\partial w_j^{(2)}} = (\hat{y} - y) \frac{\partial \hat{y}}{\partial w_j^{(2)}} = (\hat{y} - y) \sum_i x_i w_{ij}^{(1)}$$

- For the first layer (connecting inputs to hidden):

$$\frac{\partial \mathcal{L}}{\partial w_{ij}^{(1)}} = \left(\frac{\partial \mathcal{L}}{\partial \hat{y}} \frac{\partial \hat{y}}{\partial w_j^{(2)}} \right) \frac{\partial h_j}{\partial w_{ij}^{(1)}} = \left(\frac{\partial \mathcal{L}}{\partial \hat{y}} \frac{\partial \hat{y}}{\partial w_j^{(2)}} \right) x_i$$

where $h_j = x_i w_{ij}^{(1)}$ is the output of the hidden layer

Bias terms

- The toy example did not include bias terms, but these are very important (as seen in the perceptron examples)
- With a single layer we can add a column of 1s to $\mathbf{X}$, but with multiple layers we need to add bias at **every layer**
- The forward pass becomes:

$$\hat{\mathbf{y}} = (\mathbf{X}\mathbf{W}^{(1)} + \mathbf{b}^{(1)})\mathbf{W}^{(2)} + \mathbf{b}^{(2)}$$

- The calculation of the gradient is fortunately unaffected, but network size increases as weights for the bias terms need to be updated as well

Computational considerations

- Many of the terms computed in the **forward pass** are reused in the **backward pass**
- Similarly, gradients computed in layer $l+1$ are reused in layer l
- Typically each intermediate value is stored, but modern networks are **big**

Model	Parameters
Our example	6
AlexNet (2012)	60 million
GPT-3 (2020)	175 billion

Choices in neural network design

Activation functions

- The simple example used a **linear activation function** (identity)
- To include other activation functions, the forward pass becomes:

$$\hat{\mathbf{y}} = \mathbf{f_2}(\mathbf{f_1}(\mathbf{X}\mathbf{W}^{(1)})\mathbf{W}^{(2)})$$

- The gradient in the output layer becomes:

$$\frac{\partial \mathcal{L}}{\partial w_j^{(2)}} = \frac{\partial \mathcal{L}}{\partial f_2} \frac{\partial f_2}{\partial \hat{y}} \frac{\partial \hat{y}}{\partial w_j^{(2)}}$$

- Problem! That step function in the original perceptron is not differentiable

Activation functions

- A common early choice was the sigmoid function:

$$\sigma(z) = \frac{1}{1+e^{-z}}, \qquad \frac{d\sigma}{dz} = \sigma(z)(1-\sigma(z))$$

- A more computationally efficient choice common today is the "ReLU" (Rectified Linear Unit) function:

$$\mathrm{ReLU}(z) = \max(0, z), \qquad \frac{d\mathrm{ReLU}}{dz} = \begin{cases} 0 & z < 0 \\ 1 & z > 0 \end{cases}$$

- What about $z = 0$? Most implementations just set it to 0

Activation functions in hidden layers

> *The design of hidden units is an extremely active area of research and does not yet have many definitive guiding theoretical principles.*
> *-- Deep Learning Book, Section 6.3*

- Activation functions in hidden layers serve to **introduce nonlinearity**
- Common for multiple hidden layers to use the same activation function
- Sigmoid, ReLU, and tanh (hyperbolic tangent) are common choices
- Also "leaky" ReLU, Parameterized ReLU, absolute value, etc
- Can be considered a **hyperparameter** of the network

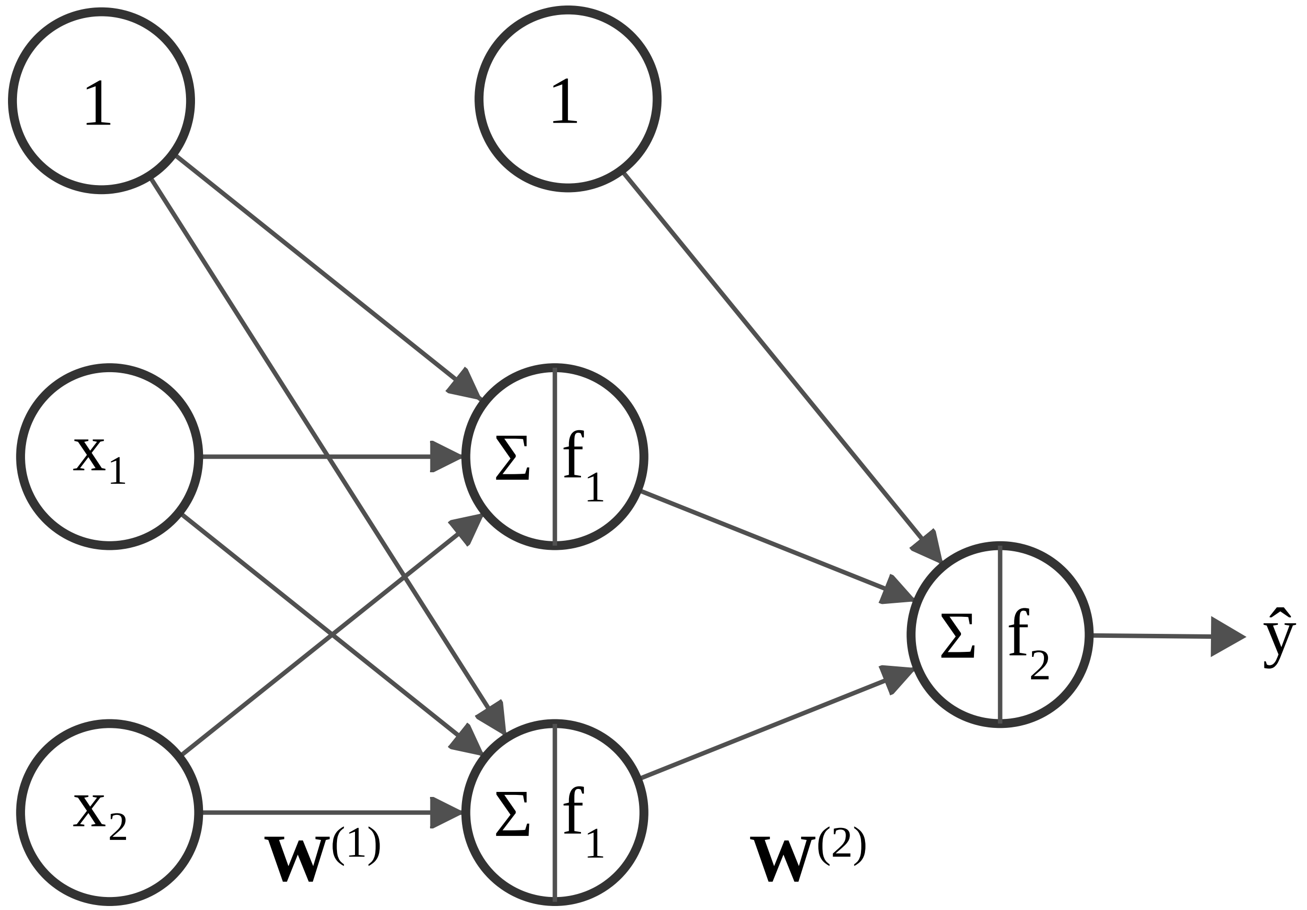
Loss functions

- The choice of loss function is very important!
- Depends on the task at hand, e.g.:
  - Regression: MSE, MAE, etc
  - Classification: Usually some kind of cross-entropy (log likelihood)
- May or may not include regularization terms
- Must be differentiable, just like the activation functions

Activation functions in the output layer

- Activation functions in the **output** layer should be chosen based on the loss function (and thus the task)
  - Regression: linear
  - Binary classification: sigmoid
  - Multiclass classification: softmax (generalization of sigmoid)
- Again, must be differentiable

A complete fully connected network



Next up: Classification loss functions and metrics