Machine Learning

Advanced Neural Networks

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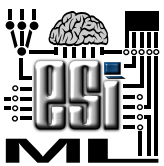

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Machine Learning

Advanced Neural Networks: Motivation

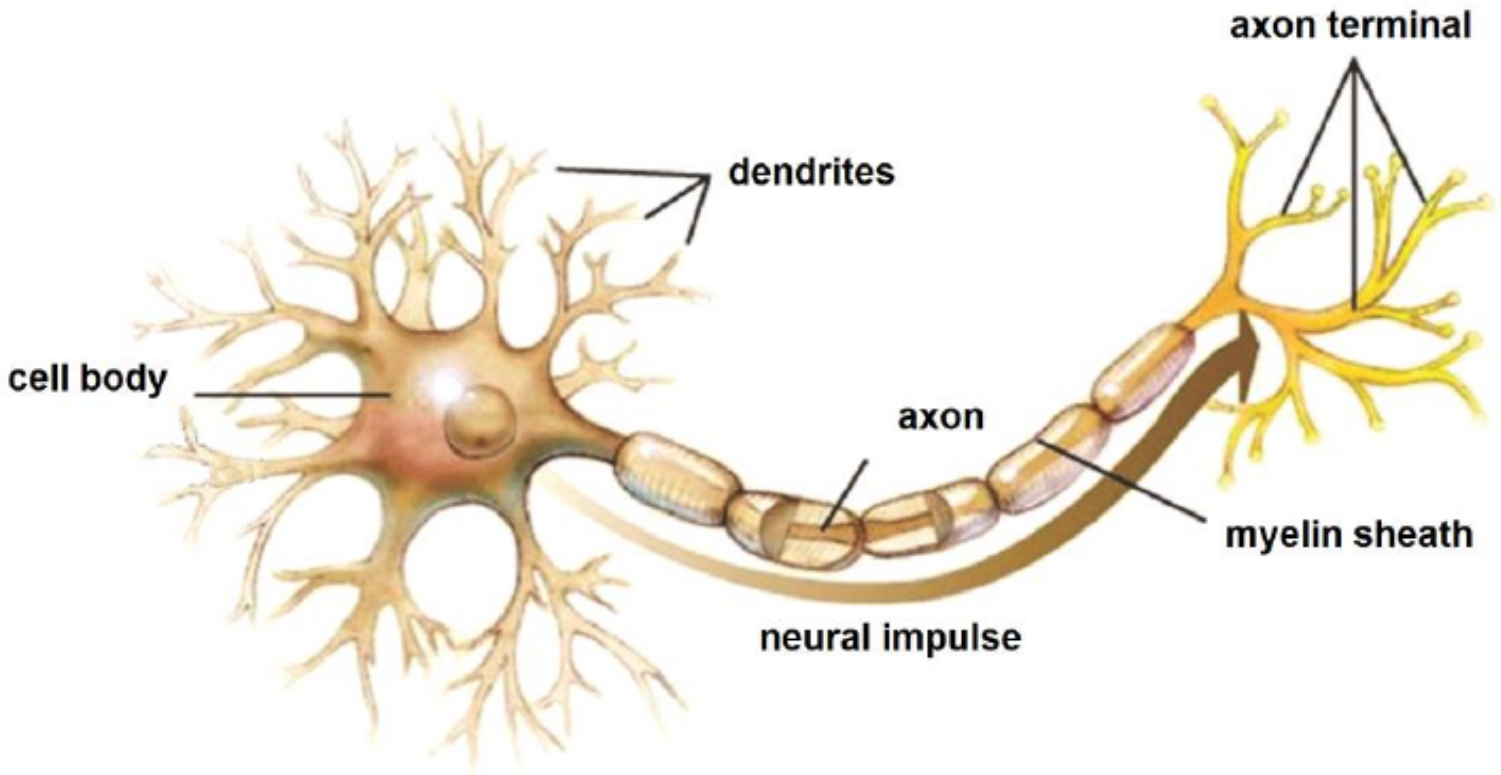


Figure: Biological neuron **[Cain, 2017]**

Machine Learning

Advanced Neural Networks: Network types

Neural Networks

Feed Forward (FFNN)

MultiLayer Perceptron (MLP)

- Dense (Fully connected)
- Embedding
- Droupout
- Layer normalization
- Batch normalization

Convolutional (CNN)

- Conv
- Pooling (max, avg)
- Flatten
- Up-sampling

Attention

- Dot-product (Luong)
- Additive (Bahdanau)
- Transformer

Recurrent (RNN)

Vanilla RNN

- Elman network
- Jordan network

Advanced RNN

- Long short-term memory (LSTM)
- Gated recurrent unit (GRU)

Energy based model (EBM)

- Hopfield network
- Boltzmann machine

Differentiable neural computers

- Neural Turing Machine (NTM)

Arch

- Encoder-Decoder
- Auto-encodeur
- Generative adversarial network (GAN)
- Deep Belief Network
- Graph neural network

Machine Learning

Advanced Neural Networks: Plan

1. **Neuron**
   - Network
   - Activation functions
   - Cost functions
   - Optimization function
2. **Feedforward Neural Networks (FFNN)**
   - Multi-layers architecture
   - Auto-encoders
   - Convolutional Neural Network (CNN)
   - Regularization
3. **Recurrent Neural Networks (RNN)**
   - Architecture (RNN)
   - Long Short-Term Memory (LSTM)
   - Gated Recurrent Unit (GRU)
4. **Attention**
   - Attention mechanism
   - Multi-Head Attention
   - Self-attention
   - Transformer

Section 1

Neuron

Advanced Neural Networks

Neuron

- Let's remember **Logistic regression**
- We make a linear combination of features' values: this can be seen as the accumulation of signals

$$z(x) = \theta_0 + \sum_{j=1}^{N} \theta_j x_j$$

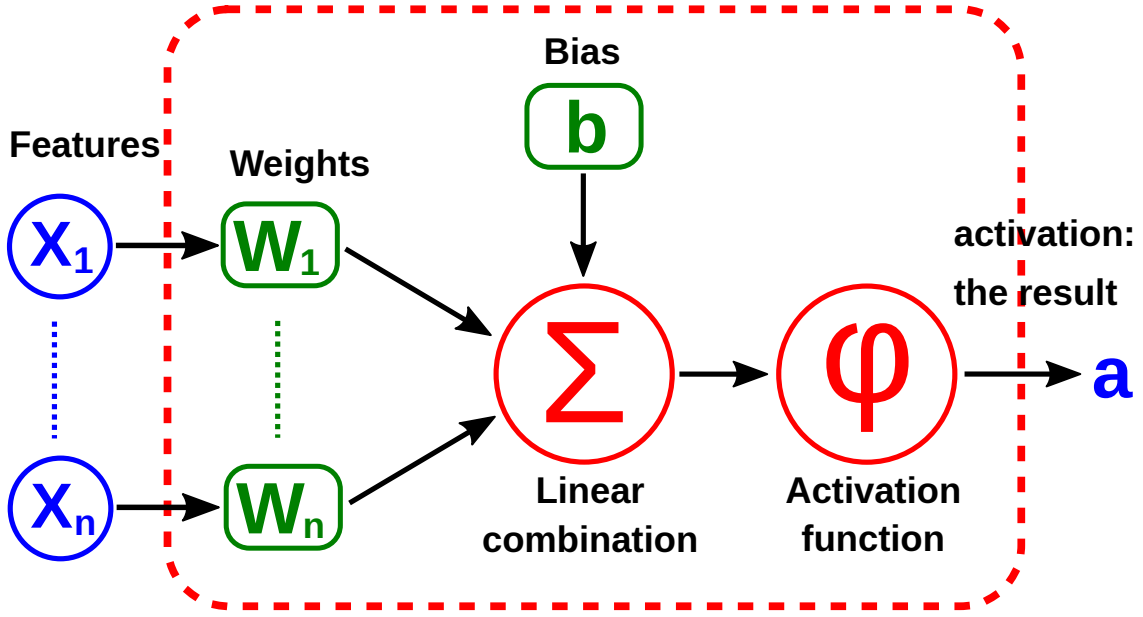
- Then, we apply the logistic function to this sum: we call it an ***activation function*** (send the signal or not according to a threshold)

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

- To calculate the classification error, we use a ***cost function***
- To train the parameters, we use an ***optimization function***

Advanced Neural Networks

Neuron

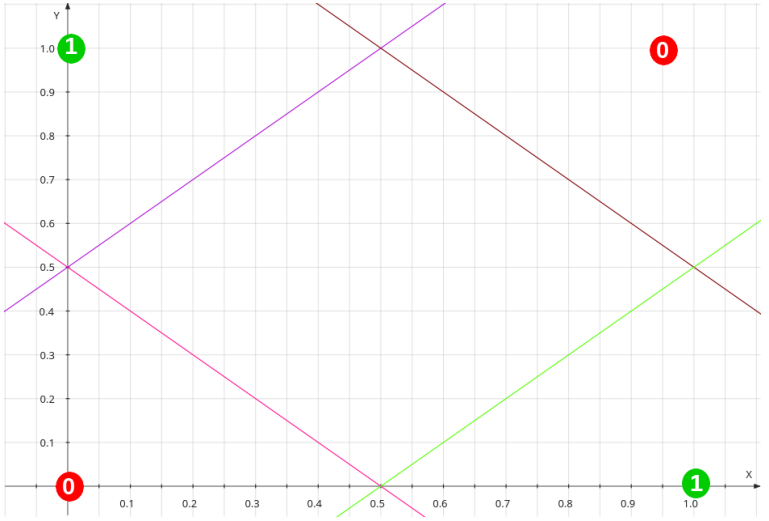


$$\hat{y} = \varphi(b + \sum_{j=1}^{n} X_j W_j)$$

Advanced Neural Networks

Neuron: Motivation

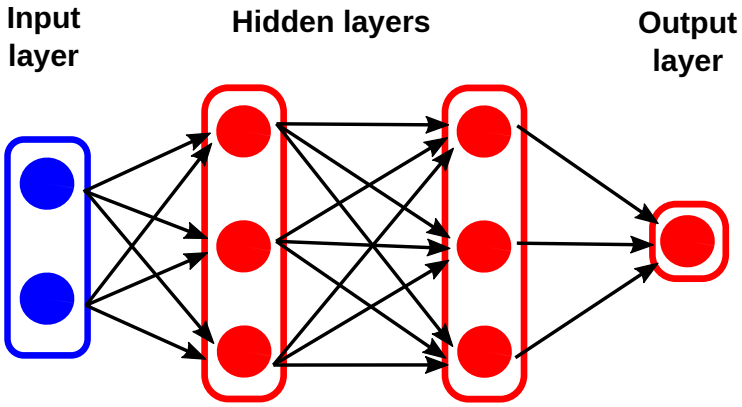
- To train complex functions, a single neuron is not enough
- For example, Two variables' XOR function
- If we train a logistic regression model (a neuron with the logistic function as activation function), the algorithm tries to separate the samples with a decision line
- Whatever the decision line, there is at least one misclassified sample



Advanced Neural Networks: Neuron

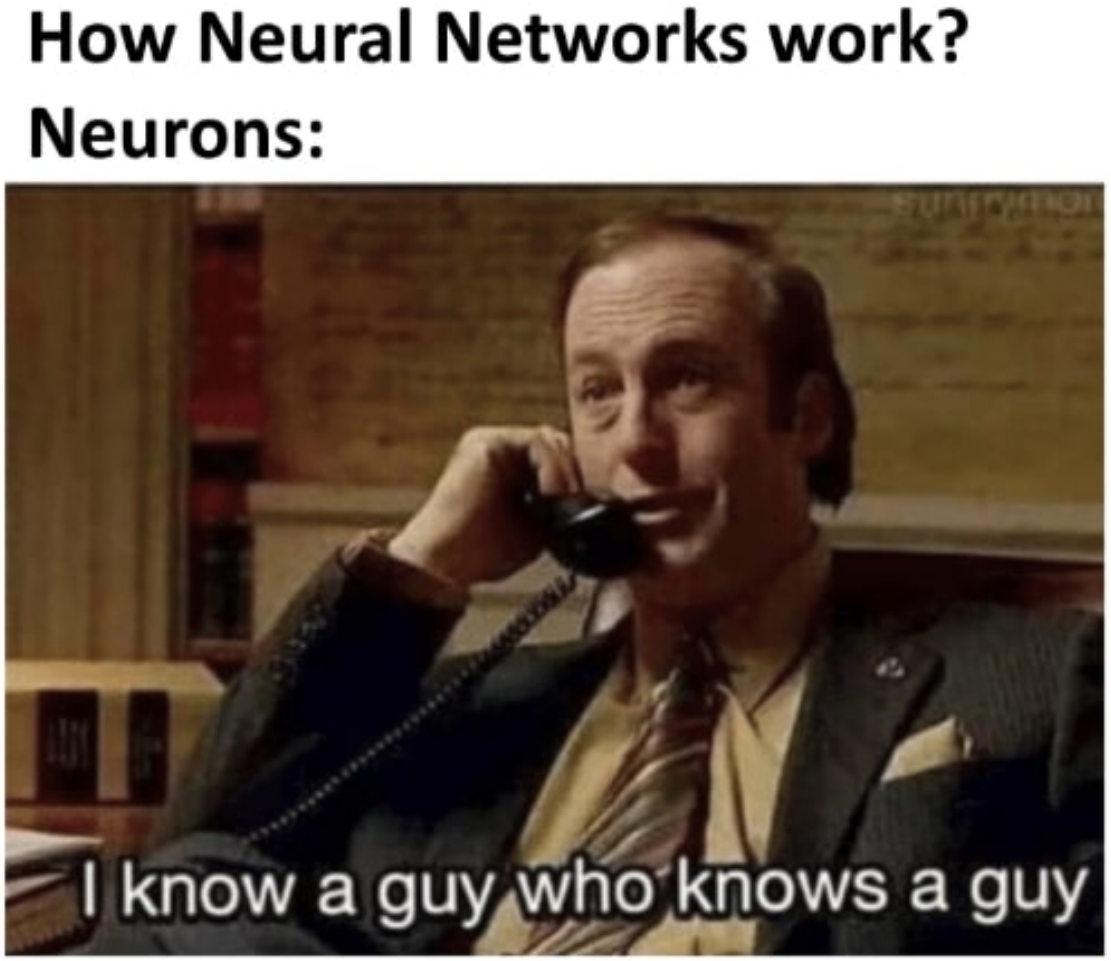
Network: Architecture

- **Input layer**: contains input values and no parameters
- **Hidden layers**: each layer receives the outputs of the previous layer. It contains a number of neurons which calculate the weighted sum with an activation function.
- **Output layer**: contains the neurons that calculate the output.



Advanced Neural Networks: Neuron

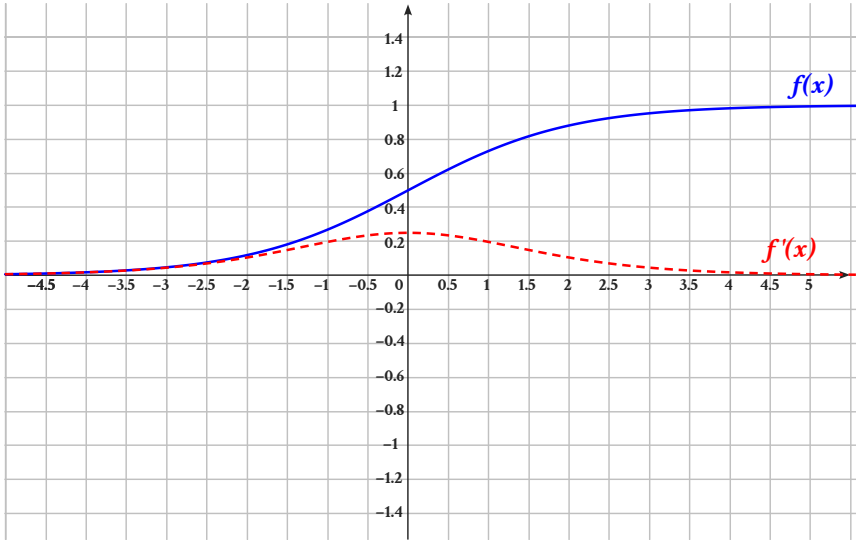
Network: Some humor



Advanced Neural Networks: Neuron

Activation functions: Sigmoid functions

Logistic function

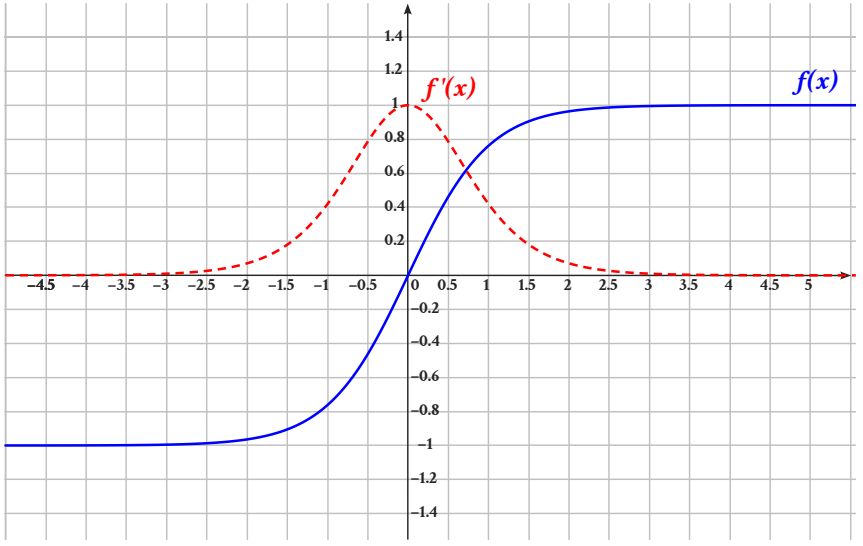


$$\sigma(x) = \frac{1}{1+e^{-x}}$$

$$\sigma(x) \in]0, 1[$$

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

Hyperbolic tangent



$$tanh(x) = \frac{e^{x}-e^{-x}}{e^{x}+e^{-x}} = \frac{2}{1+e^{-2x}} - 1$$

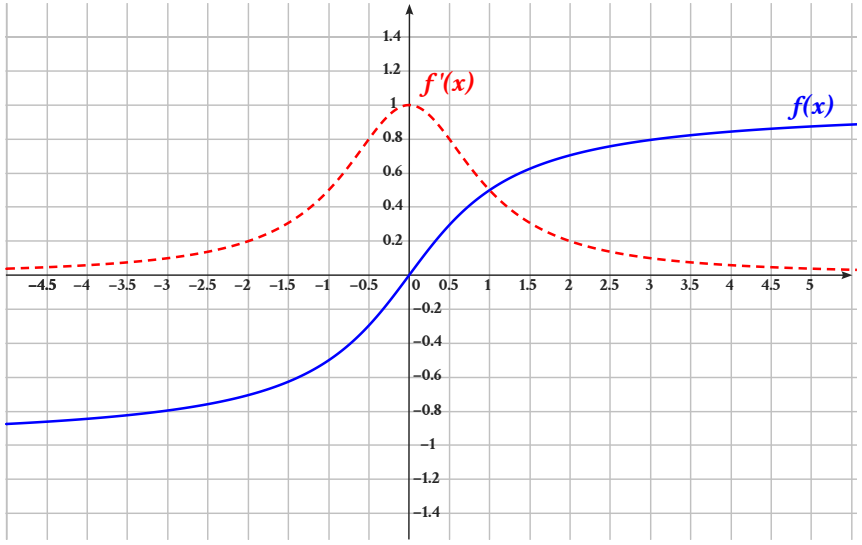
$$tanh(x) \in]-1, 1[$$

$$tanh'(x) = 1 - tanh(x)^2$$

Advanced Neural Networks: Neuron

Activation functions: Sigmoid functions (2)

Arc tangent

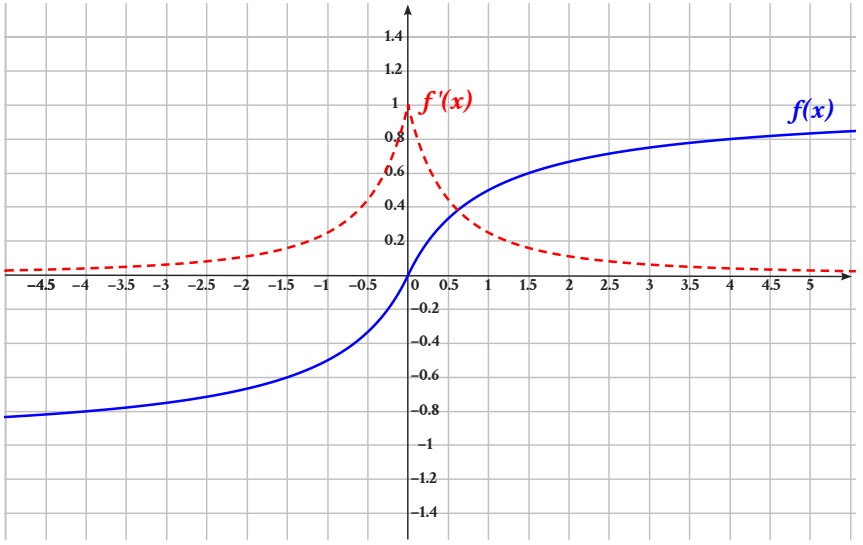


$$f(x) = \frac{2}{\pi} tan^{-1}(x)$$

$$f(x) \in]-1, 1[$$

$$f'(x) = \frac{2}{\pi} \frac{1}{x^2+1}$$

Softsign



$$f(x) = \frac{x}{1+|x|}$$

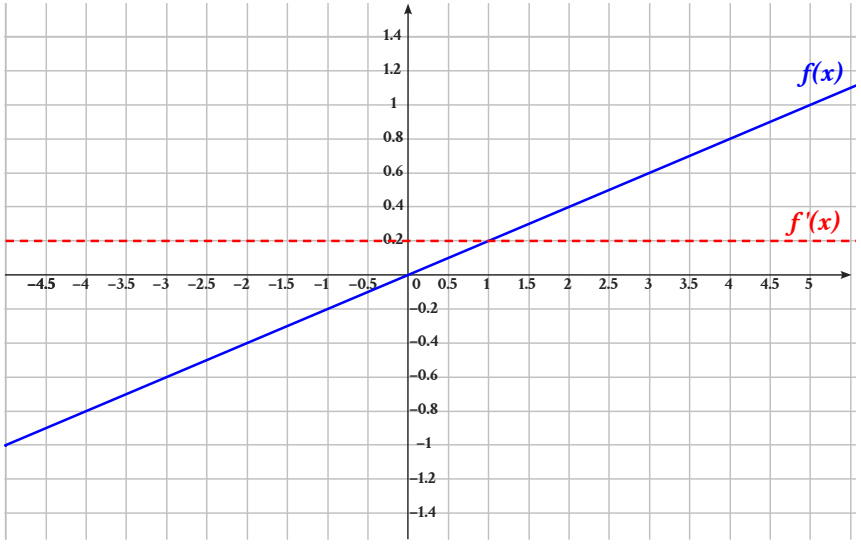
$$f(x) \in]-1, 1[$$

$$f'(x) = \frac{1}{(1+|x|)^2}$$

Advanced Neural Networks: Neuron

Activation functions: Linear functions

Linear function

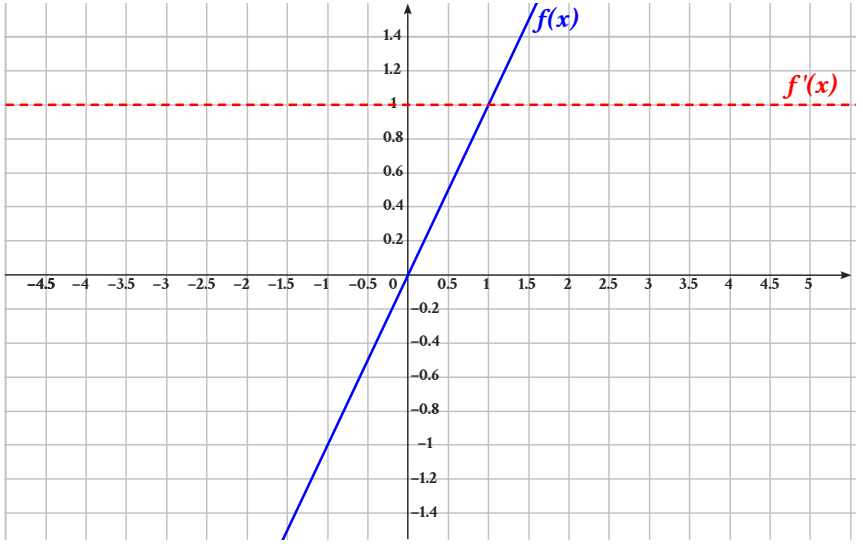


$$f(x) = kx$$

$$f(x) \in]-\infty, +\infty[$$

$$f'(x) = k$$

Identity function



$$f(x) = x$$

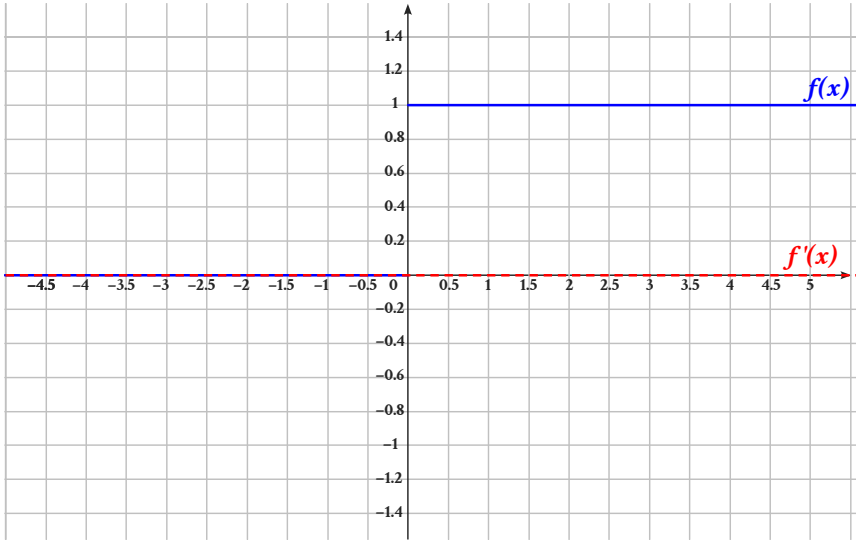
$$f(x) \in]-\infty, +\infty[$$

$$f'(x) = 1$$

Advanced Neural Networks: Neuron

Activation functions: Step functions

Heaviside function

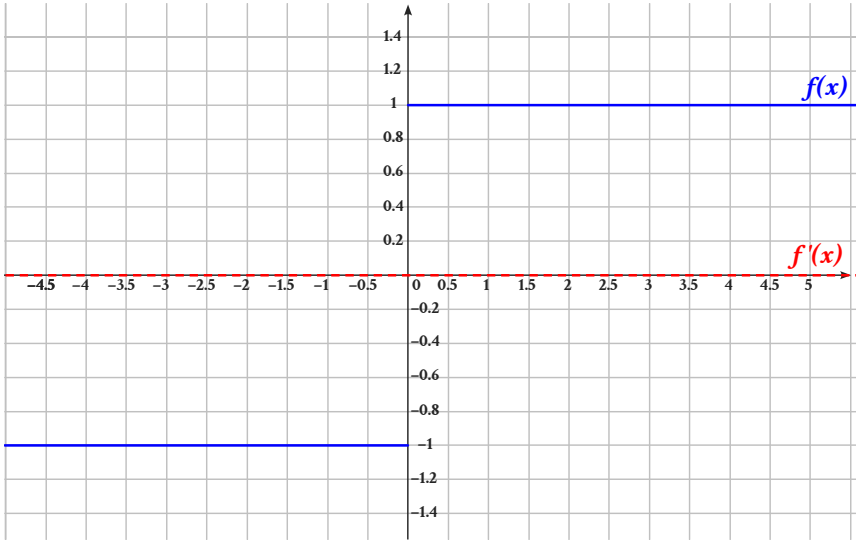


$$H(x) = \begin{cases} 0 & \text{if } x < 0 \\ 1 & \text{otherwise} \end{cases}$$

$$H(x) \in \{0, 1\}$$

$$H'(x) = \begin{cases} 0 & \text{if } x \neq 0 \\ +\infty & \text{otherwise} \end{cases}$$

Sign function



$$S(x) = \begin{cases} -1 & \text{if } x < 0 \\ 1 & \text{otherwise} \end{cases} = 2H(x) - 1$$

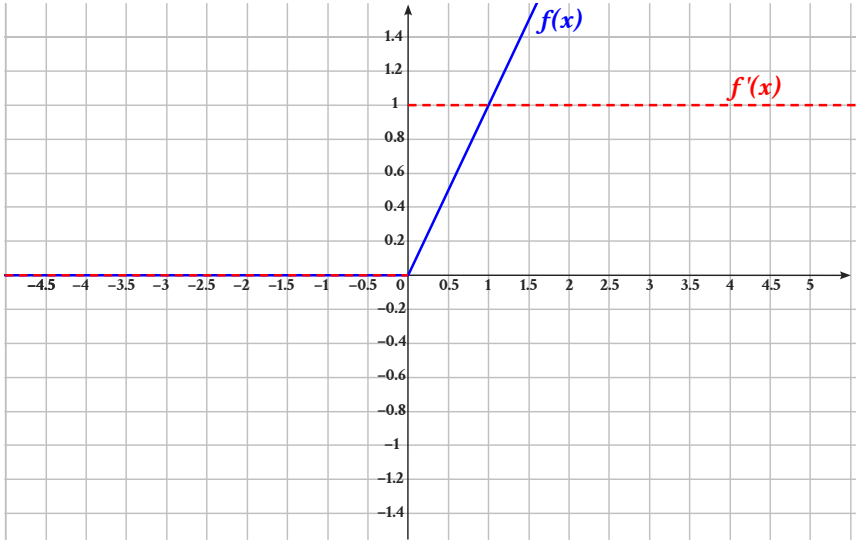
$$S(x) \in \{-1, 1\}$$

$$S'(x) = 2H'(x)$$

Advanced Neural Networks: Neuron

Activation functions: Hockey stick functions

Rectified Linear Unit

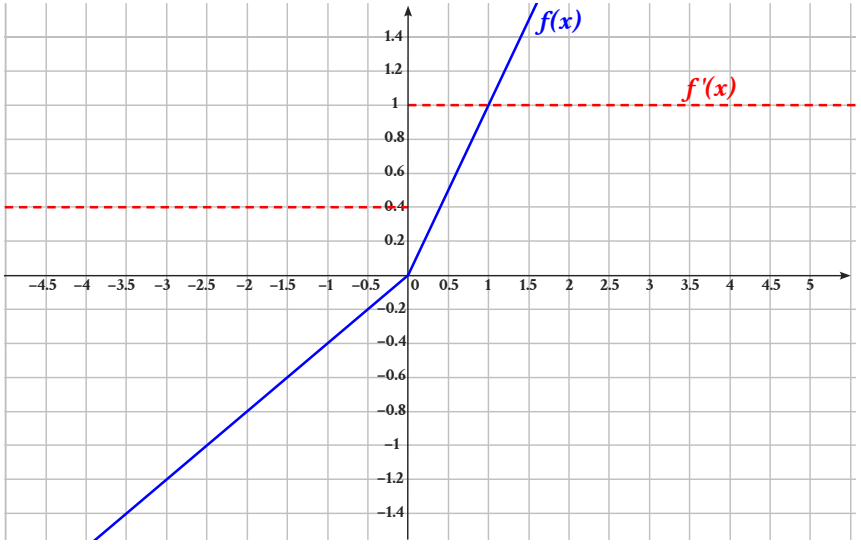


$$ReLU(x) = xH(x) = \max(0, x)$$

$$ReLU(x) \in [0, +\infty[$$

$$ReLU'(x) = H(x) = \begin{cases} 0 & \text{if } x < 0 \\ 1 & \text{otherwise} \end{cases}$$

Parametric ReLU



$$PReLU(\alpha, x) = \begin{cases} \alpha x & \text{if } x < 0 \\ x & \text{otherwise} \end{cases}$$

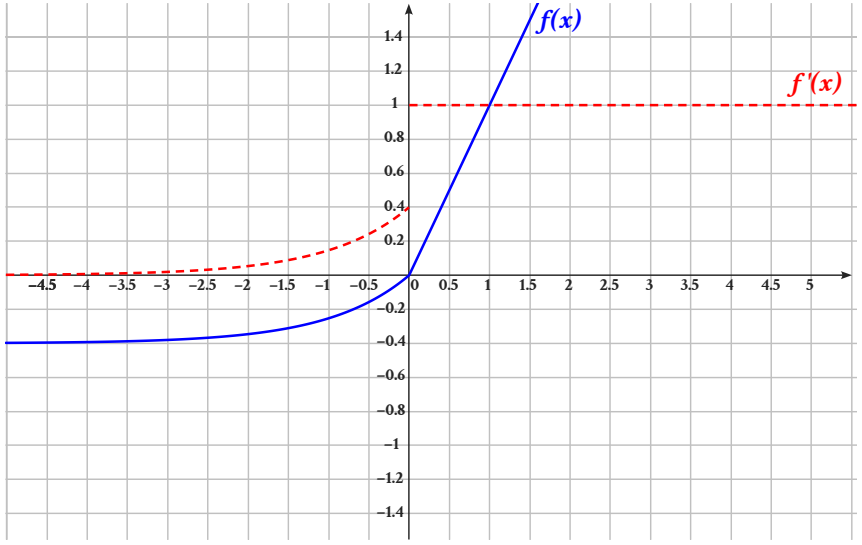
$$PReLU(x) \in]-\infty, +\infty[$$

$$PReLU'(x) = \begin{cases} \alpha & \text{if } x < 0 \\ 1 & \text{otherwise} \end{cases}$$

Advanced Neural Networks: Neuron

Activation functions: Hockey stick functions (2)

Exponential Linear Unit

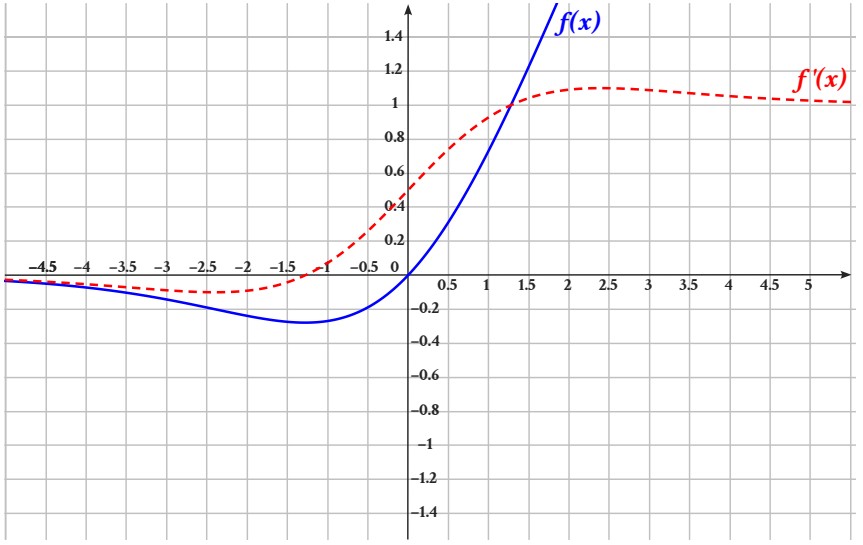


$$ELU(\alpha, x) = \begin{cases} \alpha(e^x - 1) & \text{if } x < 0 \\ x & \text{otherwise} \end{cases}$$

$$ELU(\alpha, x) \in]-\infty, +\infty[$$

$$ELU'(\alpha, x) = \begin{cases} ELU(\alpha, x) + \alpha & \text{if } x < 0 \\ 1 & \text{otherwise} \end{cases}$$

Sigmoid Linear Unit



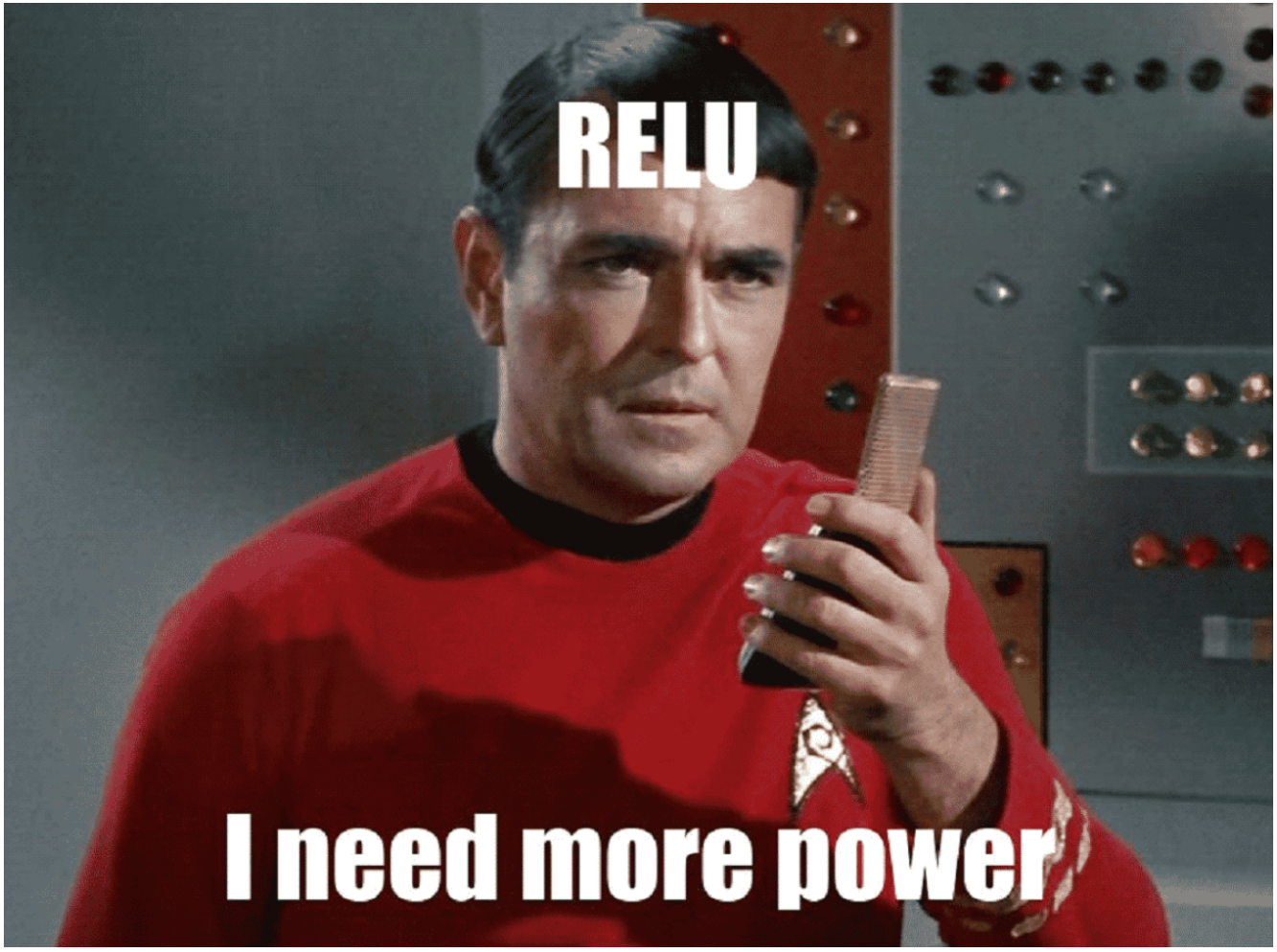
$$SLU(x) = x\sigma(x) = \frac{x}{1+e^{-x}}$$

$$SLU(x) \in]-\infty, +\infty[$$

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

Advanced Neural Networks: Neuron

Activation functions: Some humor



Advanced Neural Networks: Neuron

Cost functions: Regression (MSE)

Mean Squared Error, L2 loss

$$MSE = \frac{1}{2}(y - \hat{y})^2$$

$$\frac{\partial MSE}{\partial \hat{y}} = \hat{y} - y$$

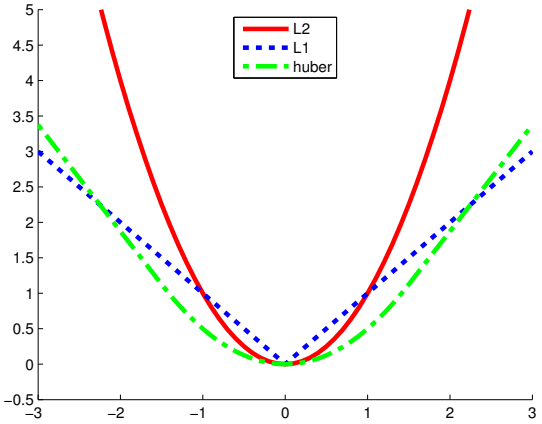


Figure: Regression cost functions **[Rosenberg, 2017]**

Advanced Neural Networks: Neuron

Cost functions: Regression (MSE)

- **Advantages**
  - A quadratic function has only one global minimum.
- **Disadvantages**
  - MSE is less robust to outliers.

Advanced Neural Networks: Neuron

Cost functions: Regression (MAE)

Mean Absolute Error, L1 loss

$$MAE = |y - \hat{y}|$$

$$\frac{\partial MAE}{\partial \hat{y}} = \begin{cases} +1 & \text{if } \hat{y} > y \\ -1 & \text{if } \hat{y} < y \\ [-1, +1] & \text{if } \hat{y} = y \end{cases}$$

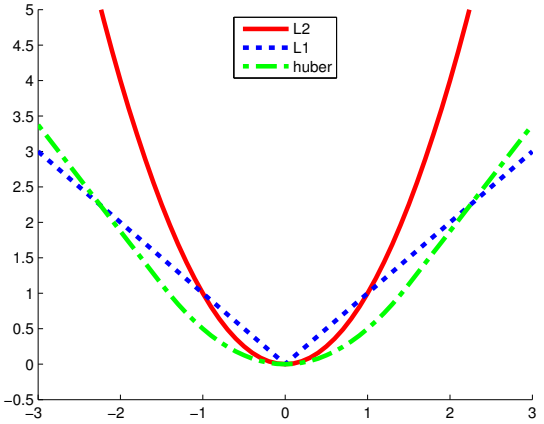


Figure: Regression cost functions **[Rosenberg, 2017]**

Advanced Neural Networks: Neuron

Cost functions: Regression (MAE)

- **Advantages**
  - Less sensitive to outliers
- **Disadvantages**
  - The amplitude of the gradient does not depend on the size of the error, only on the sign of y - ŷ. This leads to the gradient magnitude being large even when the error is small

Advanced Neural Networks: Neuron

Cost functions: Regression (Huber)

Huber Loss

$$J = \begin{cases} \frac{1}{2}(y - \hat{y})^2 & \text{if } |y - \hat{y}| \leq \delta \\ \delta|y - \hat{y}| - \frac{1}{2}\delta^2 & \text{otherwise} \end{cases}$$

$$\frac{\partial J}{\partial \hat{y}} = \begin{cases} \hat{y} - y & \text{if } |\hat{y} - y| \leq \delta \\ -\delta & \text{if } \hat{y} - y < -\delta \\ +\delta & \text{if } \hat{y} - y > \delta \end{cases}$$

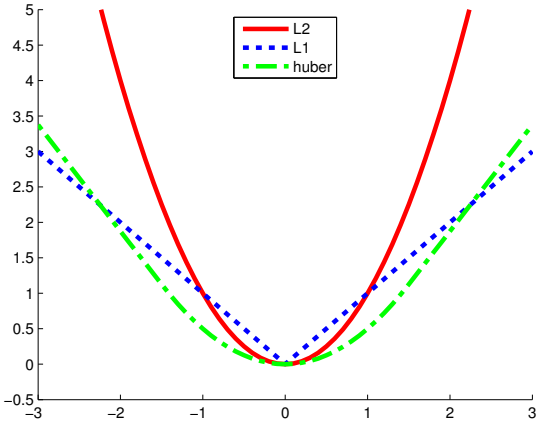


Figure: Regression cost functions **[Rosenberg, 2017]**

Advanced Neural Networks: Neuron

Cost functions: Regression (Huber)

- **Advantages**
  - Same advantages as MSE and MAE
- **Disadvantages**
  - Hyper-parameter δ must be tuned

Advanced Neural Networks: Neuron

Cost functions: Binary classification (BCE)

Binary Cross Entropy Loss

$$J = -(y \log(\hat{y}) + (1 - y) \log(1 - \hat{y}))$$

$$\frac{\partial J}{\partial \hat{y}} = \frac{\hat{y} - y}{\hat{y} - \hat{y}^2}$$

- **Advantages**
  - works well with activation functions that model probabilities (sigmoid)
  - Therefore, best estimate of the probabilities
- **Disadvantages**
  - linear separation margin is not guaranteed to be optimal

Advanced Neural Networks: Neuron

Cost functions: Binary classification (Hinge)

Hinge Loss (SVM Loss)

$$J = \max(0, 1 - y\hat{y}), y \in \{-1, 1\}$$

$$\frac{\partial J}{\partial \hat{y}} = \begin{cases} 0 & \text{if } y\hat{y} \geq 1 \\ -y & \text{otherwise} \end{cases}$$

- **Advantages**
  - results in better precision
- **Disadvantages**
  - non-smooth and non-differentiable, therefore fewer optimization algorithms
  - does not model the probability $p(y|x)$ directly

Advanced Neural Networks: Neuron

Cost functions: Multi-class classification (Cross entropy)

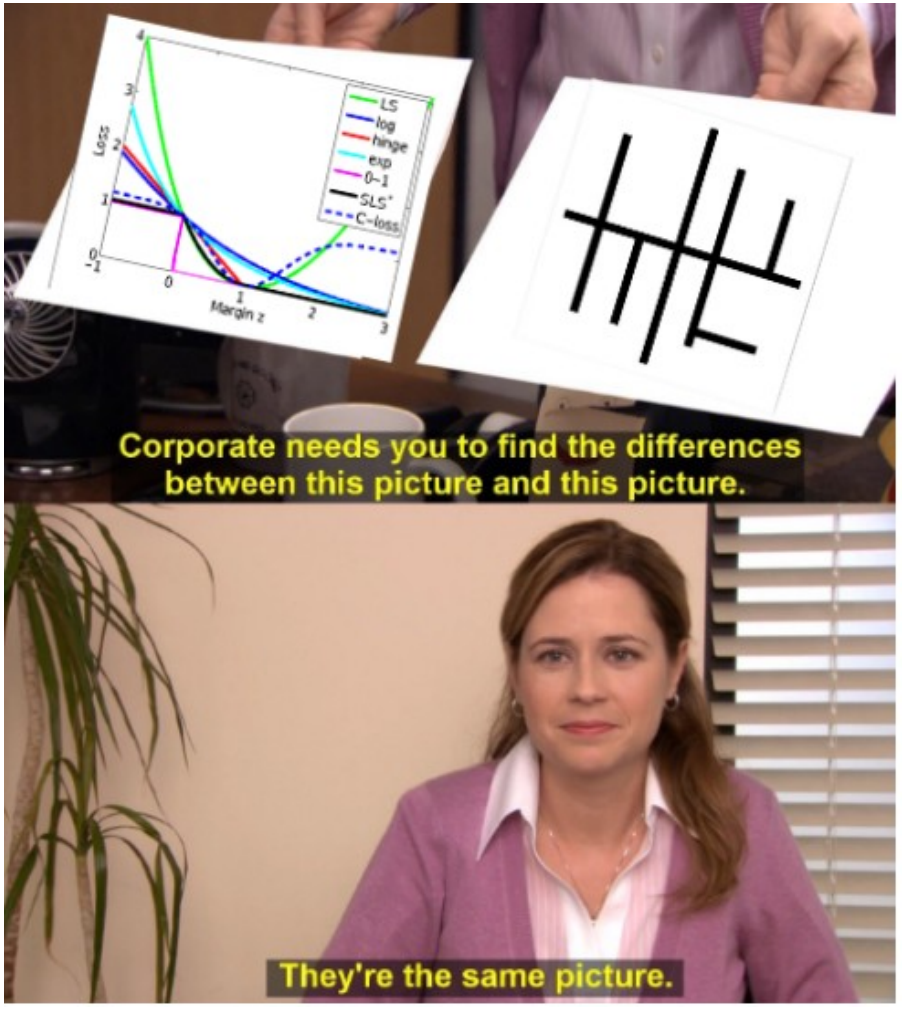
Cross Entropy Loss

$$J = -\sum_{k=1}^{K} y_k \log(\hat{y}_k), \text{ où } K \text{ est le nnombre des classes}$$

$$\frac{\partial J}{\partial \hat{y}_k} = -\frac{y_k}{\hat{y}_k}$$

Advanced Neural Networks: Neuron

Cost functions: Some humor



Advanced Neural Networks: Neuron

Optimization function: Gradient Descent

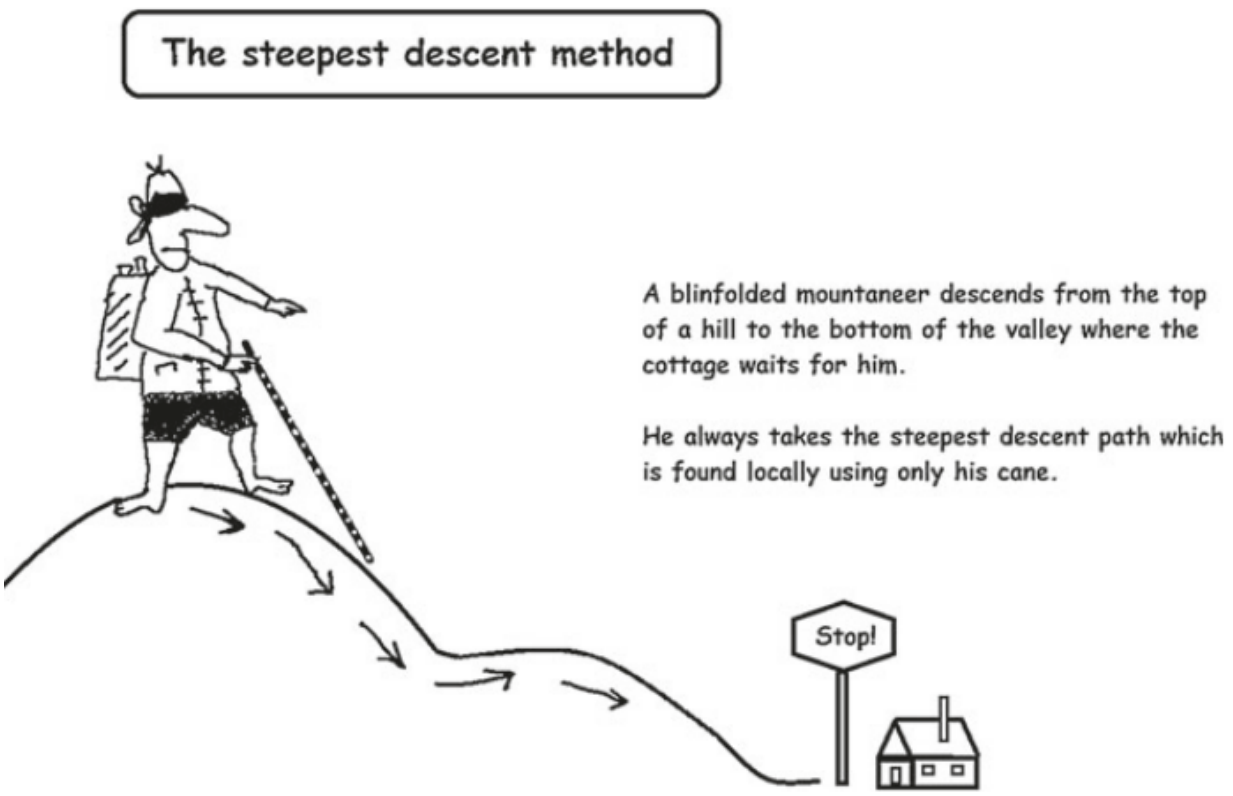


Figure: Illustration of gradient descent **[Calin, 2020]**

Advanced Neural Networks: Neuron

Optimization function: Gradient Descent

Data: X, Y, α, T
Result: θ
initialize θ ; $t = 0$;
while $t < T$ *and no convergence* **do**
    $\theta = \theta - \alpha \Delta_\theta J(X, Y; \theta)$;
    t = t + 1 ;
end

Algorithm 1: Gradient Descent

Advanced Neural Networks: Neuron

Optimization function: Gradient Descent

- **Properties**:
  - Solve the optimal value in the direction of gradient descent.
  - The method converges with a linear manner.
- **Advantages**:
  - The solution is a global optimum when the objective function is convex.
- **Disadvantages**:
  - For each parameter update, the gradients of all samples must be calculated. So the computational cost is very high.
  - The entire workout may be too large to process in memory
  - can converge to a local minimum when the objective function is not convex

Advanced Neural Networks: Neuron

Optimization function: Stochastic Gradient Descent

Data: X, Y, α, T
Result: θ
initialize θ ; $t = 0$;
while $t < T$ *and no convergence* **do**
    Randomly choose $(X^{(i)}, Y^{(i)}) \in (X, Y)$;
    $\theta = \theta - \alpha \Delta_\theta J(X^{(i)}, Y^{(i)}; \theta)$;
    t = t + 1 ;
end

Algorithm 2: Stochastic Gradient Descent

Advanced Neural Networks: Neuron

Optimization function: Stochastic Gradient Descent

- **Properties**:
  - Parameters are updated based on each sample
- **Advantages**:
  - Can avoid local minima
- **Disadvantages**:
  - It is difficult for the model to converge to a minimum

Advanced Neural Networks: Neuron

Optimization function: Mini-Batch Gradient Descent

Data: X, Y, α, T, b
Result: θ
initialize θ ; $t = 0$;
while $t < T$ *et pas de convergence* **do**
    Randomly shuffle the data;
    Split the data into b batches;
    foreach $(X^b, Y^b) \in batches$ **do** $\theta = \theta - \alpha \Delta_\theta J(X^b, Y^b; \theta)$;
    // We can update the parameters with the average of the steps
    t = t + 1 ;
end

Algorithm 3: Mini-Batch Gradient Descent

Advanced Neural Networks: Neuron

Optimization function: Mini-Batch Gradient Descent

- **Properties**:
  - Training is done on subsets of the dataset
  - A hyper-parameter b for the size of a batch
- **Advantages**:
  - Can avoid local minima due to frequent updates
  - Effective in case of large training data
- **Disadvantages**:
  - An additional hyper-parameter must be configured

Advanced Neural Networks: Neuron

Optimization function: Adaptive Gradient Descent (AdaGrad)

Data: X, Y, α, T
Result: θ
initialize θ ; $t = 0$;
initialize v ($|v| = |\theta|$) to zero;
while $t < T$ *and no convergence* **do**
    $v = v + (\Delta_\theta J(X, Y; \theta))^2$;
    $\theta = \theta - \frac{\alpha}{\sqrt{v+\epsilon}} \Delta_\theta J(X, Y; \theta)$;// epsilon is used to avoid division by 0, typically 1e-8
    t = t + 1 ;
end

Algorithm 4: Adaptive Gradient Descent **[Duchi et al., 2011]**

Advanced Neural Networks: Neuron

Optimization function: Adaptive Gradient Descent (AdaGrad)

- **Properties**:
  - The learning rate is adaptively adjusted based on the sum of squares of all historical gradients.
- **Advantages**:
  - The learning rate of each parameter adjusts adaptively
- **Disadvantages**:
  - Over time, the learning rate falls toward zero; the algorithm is not desirable for non-convex functions.

Advanced Neural Networks: Neuron

Optimization function: Root Mean Square Propagation (RMSProp)

Data: X, Y, α, T, β
Result: θ
initialize θ ; $t = 0$;
initialize v ($|v| = |\theta|$) to zero;
while $t < T$ *and no convergence* **do**
  $v = \beta v + (1 - \beta)(\Delta_\theta J(X, Y; \theta))^2$;
  $\theta = \theta - \frac{\alpha}{\sqrt{v}+\epsilon} \Delta_\theta J(X, Y; \theta)$;
  t = t + 1 ;
end

Algorithm 5: RMSProp **[Hinton et al., 2014]**

Advanced Neural Networks: Neuron

Optimization function: Root Mean Square Propagation (RMSProp)

- **Properties**:
  - Change the total gradient accumulation mode to exponential moving average.
  - By default, $\beta = 0.9$
- **Advantages**:
  - Addresses the inefficient learning problem in late AdaGrad.
  - Suitable for the optimization of non-stationary and non-convex problems.
- **Disadvantages**:
  - At the end of training, the update process can be stuck around the local minimum.

Advanced Neural Networks: Neuron

Optimization function: Adaptive Moment Estimation (Adam)

Data: $X, Y, \alpha, T, \beta_1, \beta_2$
Result: θ
initialize θ ; $t = 0$;
initialize v et m ($|v| = |m| = |\theta|$) to zero;
while $t < T$ *and no convergence* **do**
  $g = \Delta_\theta J(X, Y; \theta)$;
  $m = \beta_1 m + (1 - \beta_1) g$; $\hat{m} = \frac{m}{1-\beta_1^t}$;
  $v = \beta_2 v + (1 - \beta_2) g^2$; $\hat{v} = \frac{v}{1-\beta_2^t}$;
  $\theta = \theta - \frac{\alpha \hat{m}}{\sqrt{\hat{v}} + \epsilon}$;
  t = t + 1 ;
end

Algorithm 6: Adam **[Kingma and Ba, 2015]**

Advanced Neural Networks: Neuron

Optimization function: Adaptive Moment Estimation (Adam)

- **Properties**:
  - Use of first-order and second-order moments to dynamically adjust the learning rate for each parameter.
  - Addition of bias correction.
  - Default values: $\beta_1 = 0.9, \beta_2 = 0.999$
- **Advantages**:
  - The gradient descent process is relatively stable.
  - It is suitable for most non-convex optimization problems with large datasets and high-dimensional spaces.
- **Disadvantages**:
  - The method may not converge in certain cases.

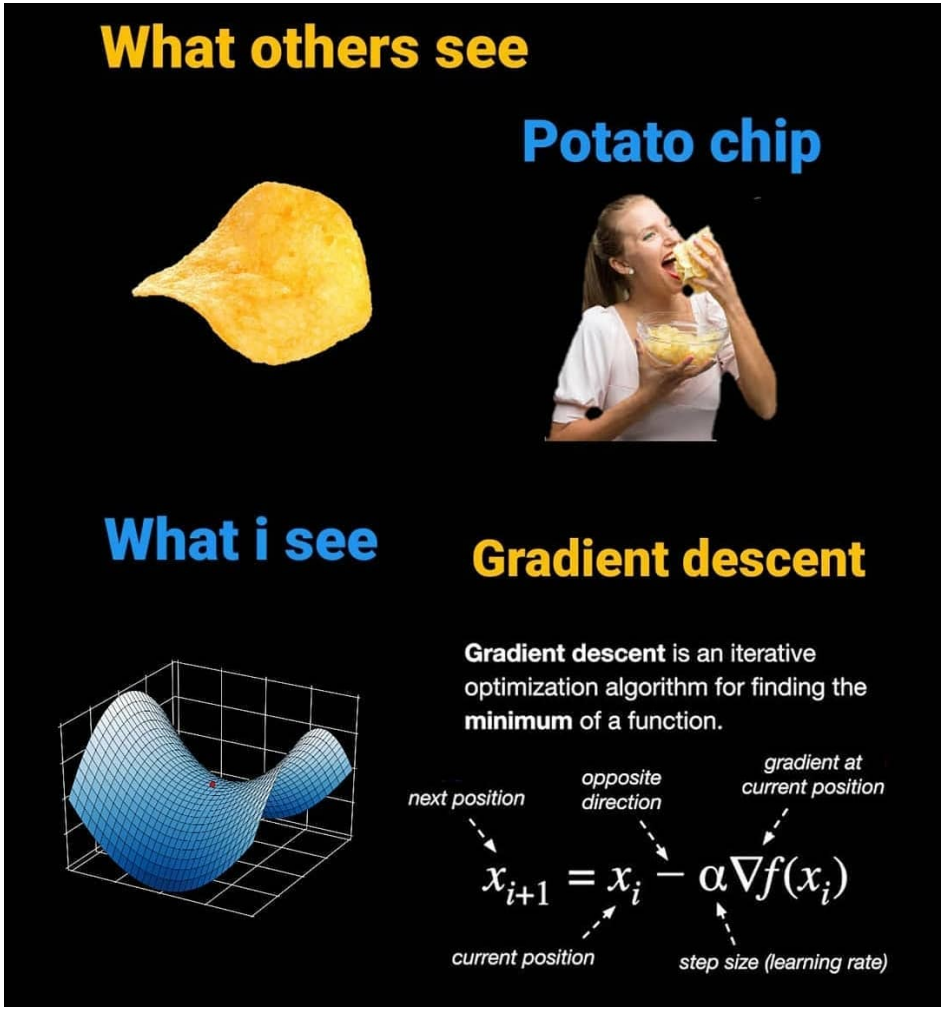
Advanced Neural Networks: Neuron

Optimization function: Others

- **COCOB [Orabona and Tommasi, 2017]**
  - https://arxiv.org/pdf/1705.07795.pdf
- **Yogi [Zaheer et al., 2018]**
  - https://proceedings.neurips.cc/paper/2018/file/90365351ccc7437a1309dc64e4db32a3-Paper.pdf
- **NovoGrad [Ginsburg et al., 2019]**
  - https://arxiv.org/pdf/1905.11286.pdf
- **Lookahead [Zhang et al., 2019]**
  - https://arxiv.org/pdf/1907.08610v1.pdf
- **LAMB [You et al., 2020]**
  - https://arxiv.org/abs/1904.00962
- **AdaBelief [Zhuang et al., 2020]**
  - https://arxiv.org/pdf/2010.07468.pdf

Advanced Neural Networks: Neuron

Optimization function: Some humor



Section 2

Feedforward Neural Networks (FFNN)

Advanced Neural Networks

Feedforward Neural Networks (FFNN)

Definition

A "Feedforward Neural Network" is an architecture of Neural Networks. In this one, there is no "feed" back from the outputs of the neurons to the inputs throughout the network. **[Sazlı, 2006]**

In other word, there is no temporal phenomena treated in the problem in question; current output does not depend on the past one.

Example

- Predicting the class of an image only based on its pixels

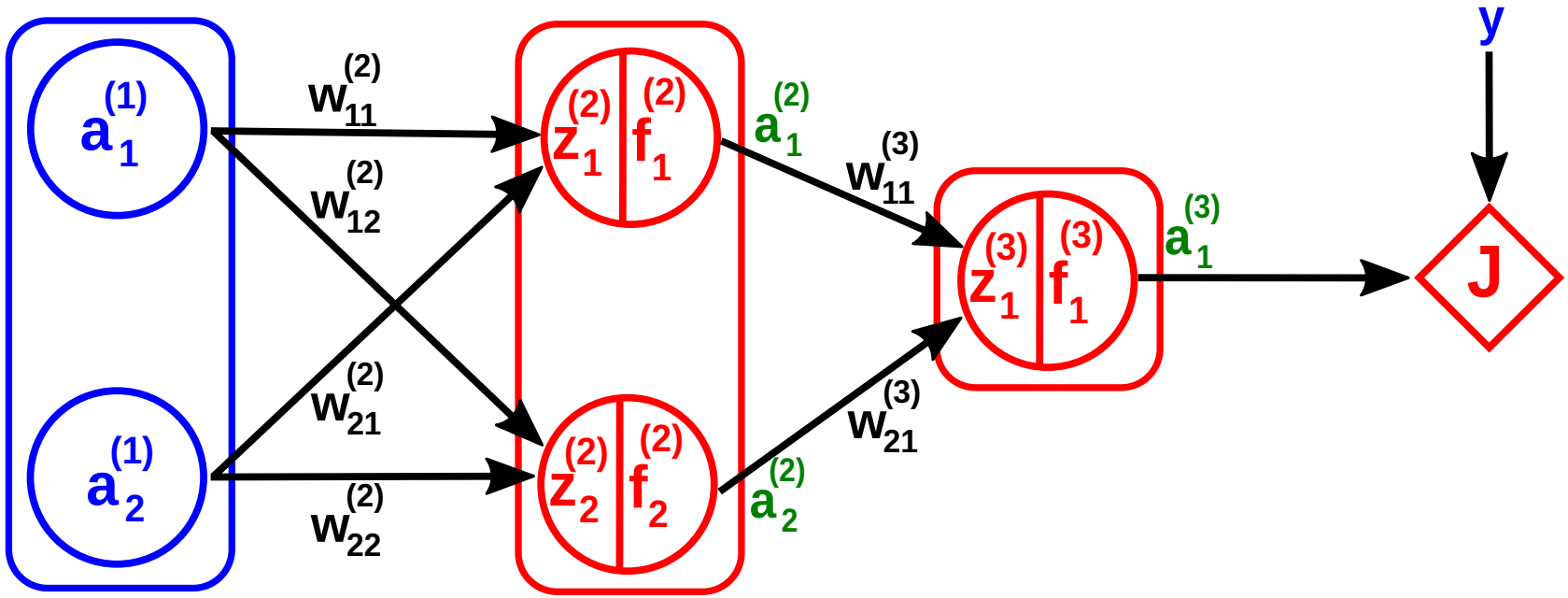
Advanced Neural Networks: Feedforward Neural Networks (FFNN)

Multi-layers architecture: Notation

$$z_j^{(l)} = \sum_i w_{ij}^{(l)} a_i^{(l-1)} + b_i^{(l)}$$

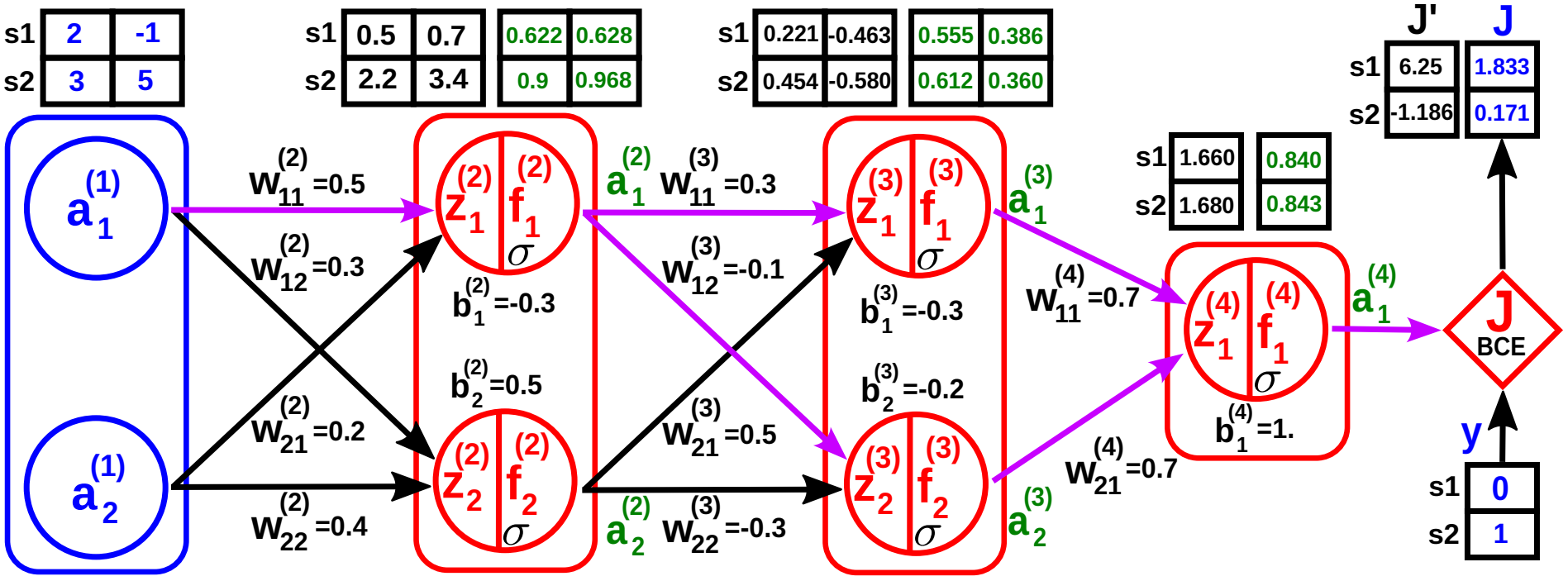
$$a_i^{(1)} = x_i$$

$$a_i^{(l)} = f_i^{(l)}(z_i^{(l)})$$



Advanced Neural Networks: Feedforward Neural Networks (FFNN)

Multi-layers architecture: Example



Advanced Neural Networks: Feedforward Neural Networks (FFNN)

Multi-layers architecture: Backpropagation [example] (1)

Update $w_{11}^{(4)}$

$$\frac{\partial J}{\partial w_{11}^{(4)}} = \overbrace{\frac{\partial J}{\partial f_1^{(4)}} \frac{\partial f_1^{(4)}}{\partial z_1^{(4)}}}^{\delta_1^{(4)}} \overbrace{\frac{\partial z_1^{(4)}}{\partial w_{11}^{(4)}}}^{a_1^{(3)}}$$

$$\frac{\partial J}{\partial f_1^{(4)}} = \frac{(0.840,0.843)-(0,1)}{(0.840,0.843)-(0.840,0.843)^2} = (6.25, -1.186)$$

$$\frac{\partial f_1^{(4)}}{\partial z_1^{(4)}} = (0.840, 0.843)(0.160, 0.157) = (0.134, 0.132)$$

$$\delta_1^{(4)} = (6.25, -1.186)(0.134, 0.132) \approx (0.838, -0.157)$$

$$\frac{\partial J}{\partial w_{11}^{(4)}} = avg((0.838, -0.157)(0.555, 0.612)) \approx avg(0.465, -0.096) = 0.184$$

$$w_{11}^{(4)} = 0.7 - 1 * (0.184) = 0.516 \text{ , supposing } \alpha = 1$$

Advanced Neural Networks: Feedforward Neural Networks (FFNN)

Multi-layers architecture: Backpropagation [example] (2)

Update $w_{21}^{(4)}$

$$\frac{\partial J}{\partial w_{21}^{(4)}} = \overbrace{\frac{\partial J}{\partial f_1^{(4)}} \frac{\partial f_1^{(4)}}{\partial z_1^{(4)}}}^{\delta_1^{(4)}} \overbrace{\frac{\partial z_1^{(4)}}{\partial w_{21}^{(4)}}}^{a_2^{(3)}}$$

$\delta_1^{(4)} = (0.838, -0.157)$

$\frac{\partial J}{\partial w_{21}^{(4)}} = avg((0.838, -0.157)(0.386, 0.360)) \approx avg(0.323, -0.056) = 0.134$

$w_{21}^{(4)} = 0.7 - 1 * (0.134) = 0.566$, supposing $\alpha = 1$

Advanced Neural Networks: Feedforward Neural Networks (FFNN)

Multi-layers architecture: Backpropagation [example] (3)

Update $w_{11}^{(3)}$

$$\frac{\partial J}{\partial w_{11}^{(3)}} = \overbrace{\underbrace{\frac{\partial J}{\partial f_1^{(4)}}}_{\delta_1^{(4)}} \underbrace{\frac{\partial f_1^{(4)}}{\partial z_1^{(4)}} \frac{\partial z_1^{(4)}}{\partial f_1^{(3)}}}_{w_{11}^{(4)}} \frac{\partial f_1^{(3)}}{\partial z_1^{(3)}}}^{\delta_1^{(3)}} \underbrace{\frac{\partial z_1^{(3)}}{\partial w_{11}^{(3)}}}_{a_1^{(2)}}$$

Here, we use the past $w_{11}^{(4)}$

$$\frac{\partial f_1^{(3)}}{\partial z_1^{(3)}} \approx (0.555, 0.612)(0.445, 0.388) = (0.247, 0.237)$$

$$\delta_1^{(3)} = (0.838, -0.157) * 0.7 * (0.247, 0.237) \approx (0.145, -0.026)$$

$$\frac{\partial J}{\partial w_{11}^{(2)}} = avg((0.145, -0.026)(0.622, 0.900)) = avg(0.090, -0.023) = 0.033$$

$$w_{11}^{(2)} = 0.3 - 1 * (0.033) = 0.267 \text{ , supposing } \alpha = 1$$

Advanced Neural Networks: Feedforward Neural Networks (FFNN)

Multi-layers architecture: Backpropagation [example] (4)

Update $w_{12}^{(3)}$

$$\frac{\partial J}{\partial w_{12}^{(3)}} = \overbrace{\underbrace{\frac{\partial J}{\partial f_1^{(4)}}}_{\delta_1^{(4)}} \underbrace{\frac{\partial f_1^{(4)}}{\partial z_1^{(4)}} \frac{\partial z_1^{(4)}}{\partial f_2^{(3)}}}_{w_{11}^{(4)}} \frac{\partial f_2^{(3)}}{\partial z_2^{(3)}}}^{\delta_2^{(3)}} \underbrace{\frac{\partial z_2^{(3)}}{\partial w_{12}^{(3)}}}_{a_1^{(2)}}$$

Here, we use use the past $w_{12}^{(4)}$

$$\frac{\partial f_2^{(3)}}{\partial z_2^{(3)}} \approx (0.386, 0.360)(0.614, 0.64) = (0.237, 0.230)$$

$$\delta_2^{(3)} = (0.838, -0.157) * 0.7 * (0.237, 0.230) \approx (0.139, -0.025)$$

$$\frac{\partial J}{\partial w_{11}^{(2)}} = avg((0.139, -0.025)(0.622, 0.900)) = avg(0.086, -0.023) = 0.032$$

$$w_{11}^{(2)} = -0.1 - 1 * (0.032) = -0.132 \text{ , supposing } \alpha = 1$$

Advanced Neural Networks: Feedforward Neural Networks (FFNN)

Multi-layers architecture: Backpropagation [example] (5)

Update $w_{11}^{(2)}$

$$\frac{\partial J}{\partial w_{11}^{(2)}} = \overbrace{\left(\delta_1^{(3)} \overbrace{\frac{\partial z_1^{(3)}}{\partial f_1^{(2)}}}^{w_{11}^{(3)}} + \delta_2^{(3)} \overbrace{\frac{\partial z_2^{(3)}}{\partial f_1^{(2)}}}^{w_{12}^{(3)}}\right)}^{\delta_1^{(2)}} \frac{\partial f_1^{(2)}}{\partial z_1^{(2)}} \overbrace{\frac{\partial z_1^{(2)}}{\partial w_{11}^{(2)}}}^{a_1^{(1)}}$$

$$\frac{\partial f_1^{(2)}}{\partial z_1^{(2)}} = (0.622, 0.900)(0.378, 0.100) = (0.235, 0.09)$$

$$\delta_1^{(2)} = ((0.145, -0.026) * (0.3) + (0.139, -0.025) * (-0.1)) * (0.235, 0.09) \approx (0.006956, -0.00047683)$$

Advanced Neural Networks: Feedforward Neural Networks (FFNN)

Multi-layers architecture: Backpropagation [General case]

- $\delta^{(l)}$ are calculated, where l is the layer's order

$$\delta^{(out)} = \frac{\partial J}{\partial f^{(out)}} \frac{\partial f^{(out)}}{\partial z^{(out)}}, \ \delta^{(l)} = \frac{\partial f^{(l)}}{\partial z^{(l)}} w^{(l+1)} \delta^{(l+1)}$$

- Gradients are calculated

$$\frac{\partial J}{\partial w^{(l)}} = a^{(l-1)} \delta^{(l)}, \ \frac{\partial J}{\partial b^{(l)}} = \delta^{(l)}$$

- Parameters are updated

$$w = w - \alpha \frac{\partial J}{\partial w^{(l)}}, \ b = b - \alpha \frac{\partial J}{\partial b^{(l)}}$$

Advanced Neural Networks: Feedforward Neural Networks (FFNN)

Multi-layers architecture: Backpropagation (Some humor)

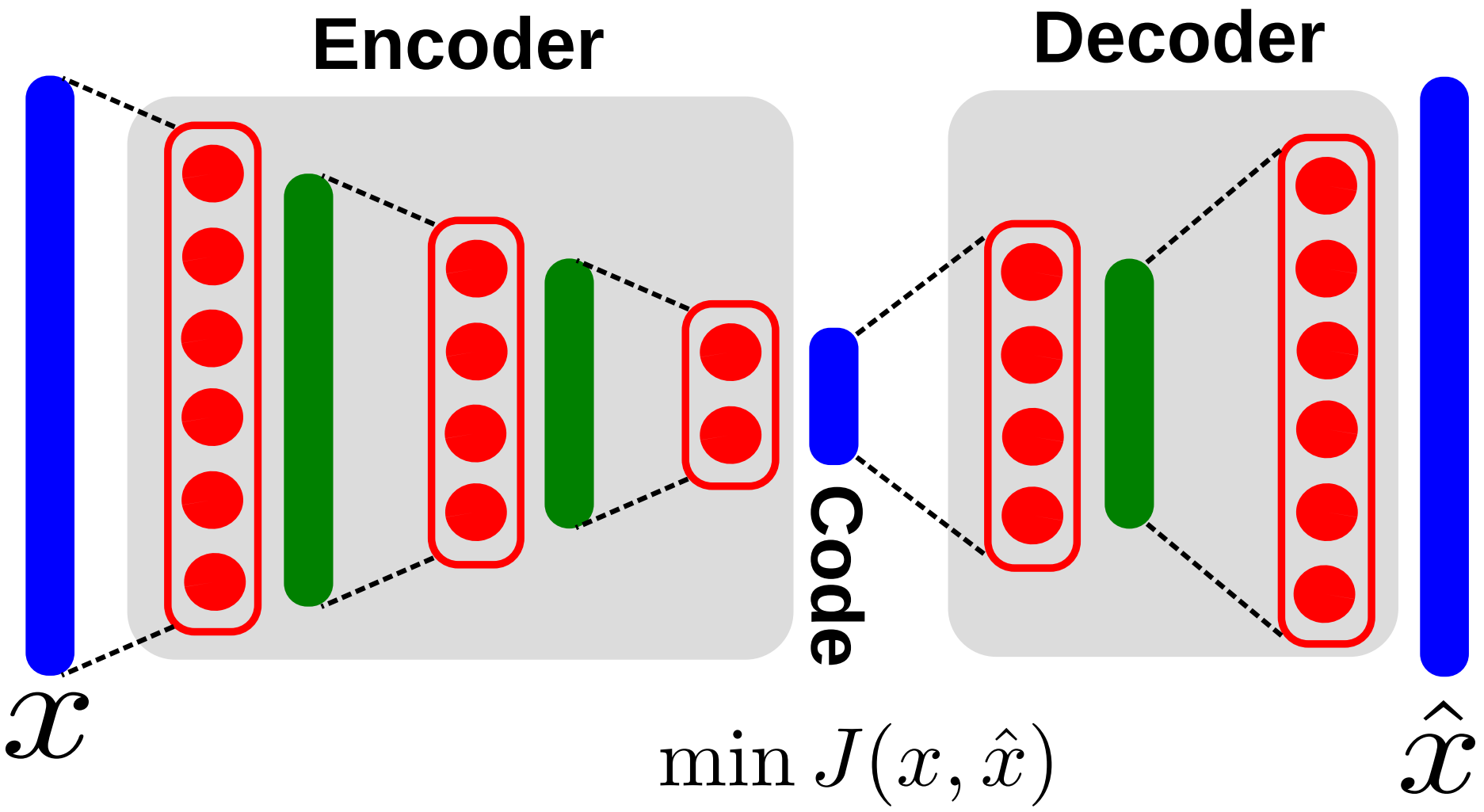
Advanced Neural Networks: Feedforward Neural Networks (FFNN)

Auto-encoders

- It is a multi-layer neural network.
- It learns a compression algorithm.
- It is characterized by **[Chollet, 2016]**:
  - Data-driven: unlike compression algorithms like JPEG.
  - Lossy data: the constructed output is not entirely identical to the input.
  - Unsupervised learning.
- It is not particularly effective for the compression task.

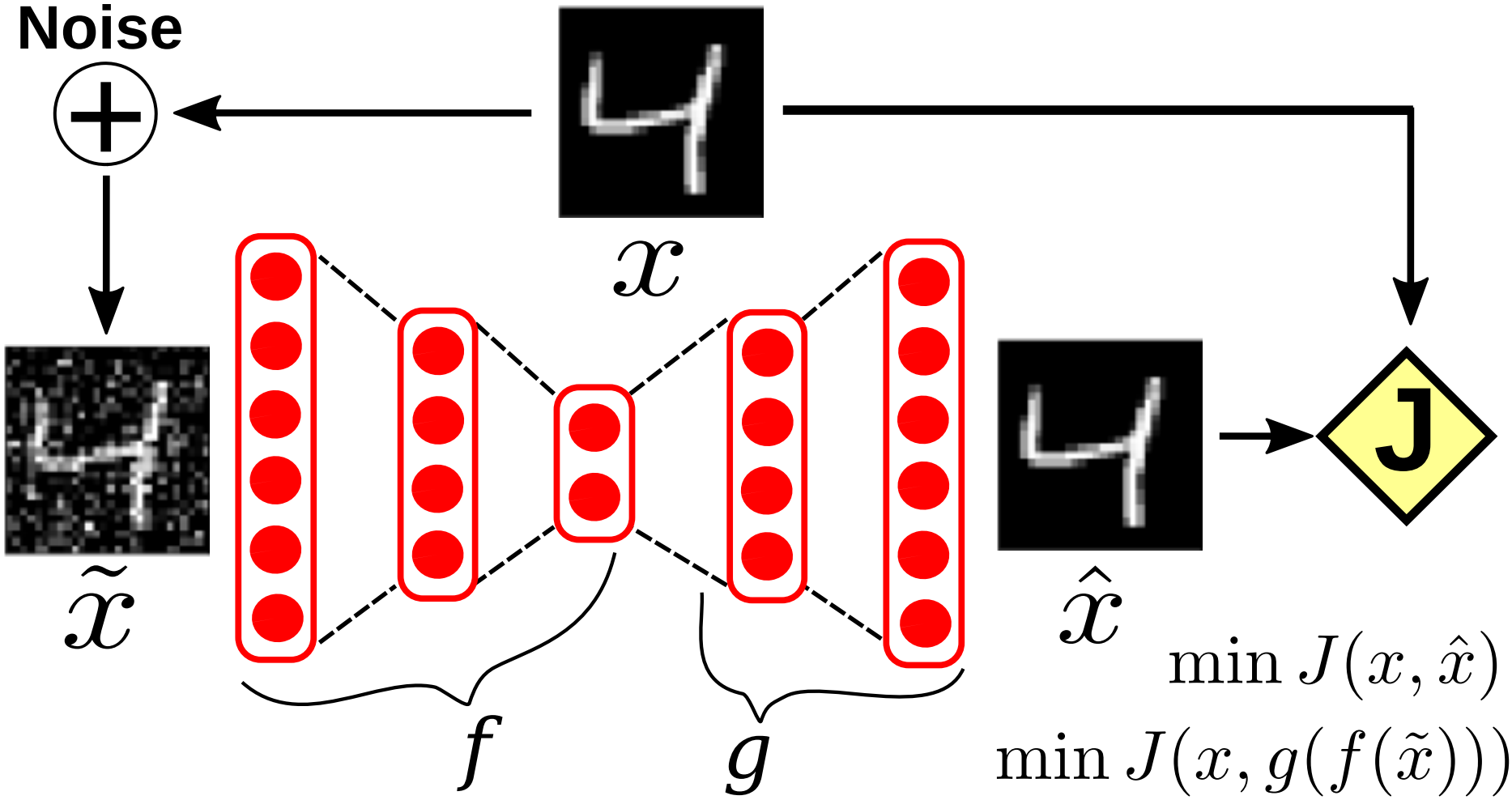
Advanced Neural Networks: Feedforward Neural Networks (FFNN)

Auto-encoders: Architecture



Advanced Neural Networks: Feedforward Neural Networks (FFNN)

Auto-encoders: Denoising Auto-encoder



Advanced Neural Networks: Feedforward Neural Networks (FFNN)

Auto-encoders: Denoising Auto-encoder (Some applications)

- Improving the quality of speech (audio) **[Lu et al., 2013]**.
- Cleaning dirty documents (refer to this competition: https://www.kaggle.com/c/denoising-dirty-documents).
- Retrieving historical documents **[Neji et al., 2019]**.
- Completing hidden parts of the face **[Li et al., 2017]**.

Advanced Neural Networks: Feedforward Neural Networks (FFNN)

Auto-encoders: Sparse Auto-encoder

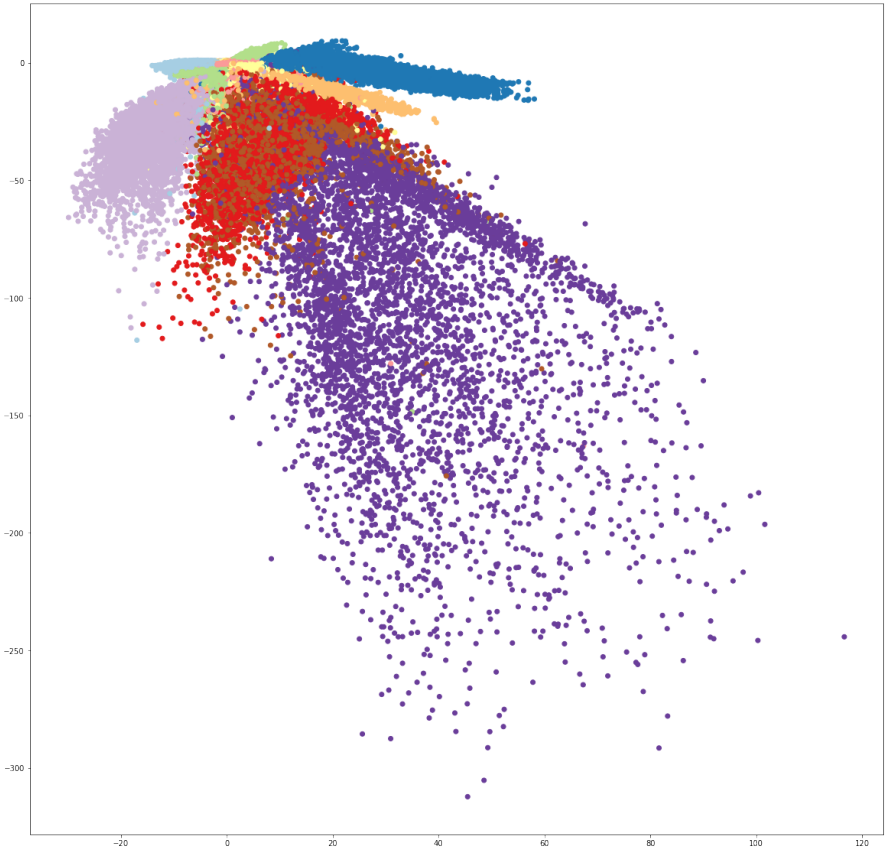
- Size of hidden layers must be equal to or larger than the input size.
- It is used to automatically learn features (feature engineering) to be used in another task, such as classification.
- Parameter (weight) regularization is applied.
- **L1** and **Kullback-Leibler divergence** are used.
- Some parameters converge to zero, allowing the learning of representations such as the contours of an object in an image.

Advanced Neural Networks: Feedforward Neural Networks (FFNN)

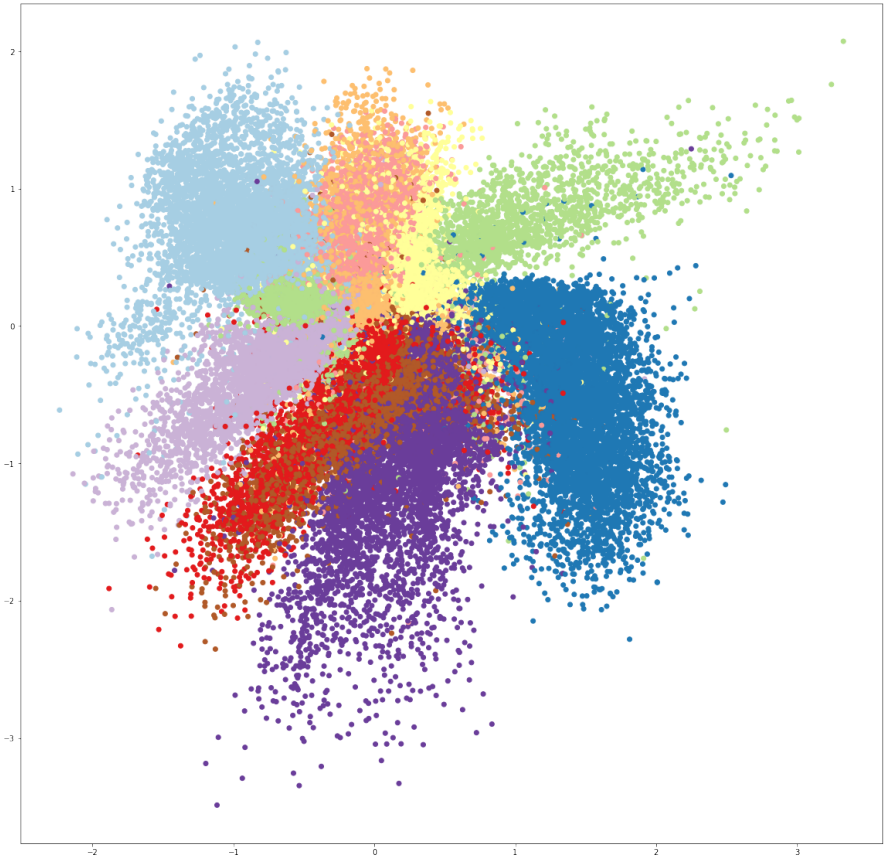
Auto-encoders: Variational Auto-encoder (Motivation)

- https://github.com/projeduc/ESI_ML/blob/main/demos/NN/TF_Autoencoder.ipynb

Clustering Auto-encoder



Variational Auto-encoder



Advanced Neural Networks: Feedforward Neural Networks (FFNN)

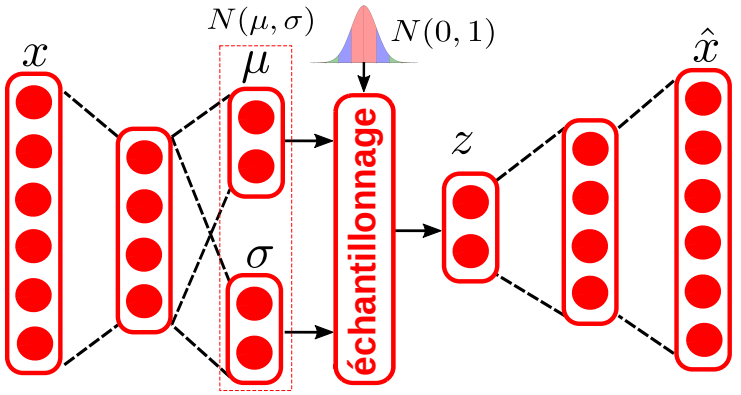
Auto-encoders: Variational Auto-encoder

- To generate new content, some random values can be input into the decoder.
- The problem is that the encoder learns to perfectly separate the different clusters.
- Solution: force the auto-encoder to learn a distribution.

$$z = \mu + \sigma * N(0,1)$$

$$J'(x,\hat{x}) = J(x,\hat{x}) + KL(N(\mu,\sigma), N(0,1))$$

$$KL(p\|q) = \sum_i p(x_i) log(\frac{p(x_i)}{q(x_i)})$$



Advanced Neural Networks: Feedforward Neural Networks (FFNN)

Auto-encoders: Variational Auto-encoder (Summary)

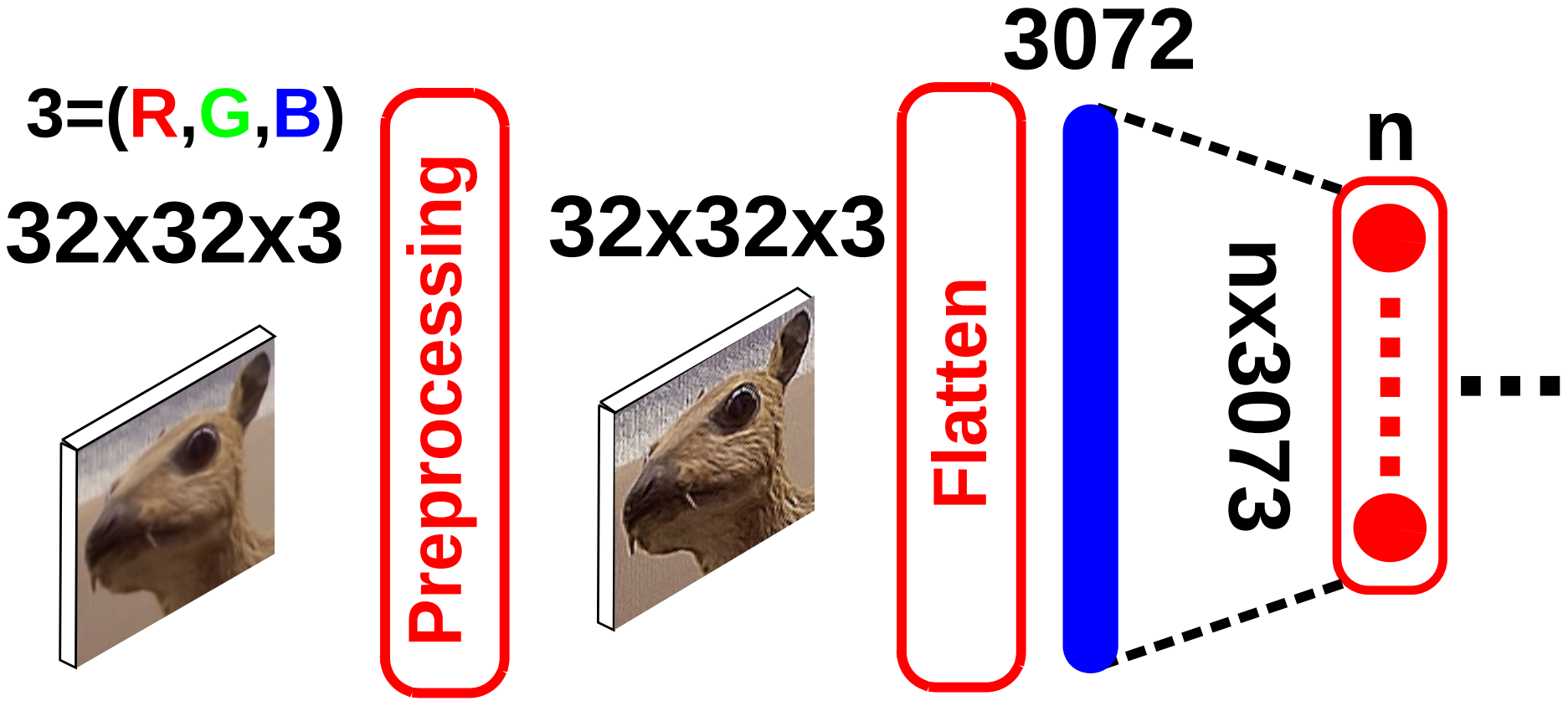
- Standard auto-encoder learns a perfect separation of clusters (non-smooth representation of latent states).
- **Solution**: force the model to learn a distribution (typically similar to the normal distribution).
- The model may learn broad distributions.
- **Solution**: use regularization (KL Divergence) to narrow them.
- The model may learn negative values for σ.
- **Solution**: learn $\log \sigma$.

Advanced Neural Networks: Feedforward Neural Networks (FFNN)

Auto-encoders: Some humor

Advanced Neural Networks: Feedforward Neural Networks (FFNN)

Convolutional Neural Network (CNN): Image processing (traditional architecture)



Advanced Neural Networks: Feedforward Neural Networks (FFNN)

Convolutional Neural Network (CNN): Image processing (preprocessing)

- There are several preprocessing techniques (see **[Alginahi, 2010]**).
- We focus on convolution-based techniques (modifying the value of a pixel relative to its neighbors).
- Two parameters: **padding** (surrounding the image with zeros to preserve the original size) and **stride** (the step size of the kernel/mask as it slides).

Original

1	2	3	4	5
6	7	8	9	0
1	3	5	7	9
0	2	4	6	8

Kernel

0	-1	0
-1	5	-1
0	-1	0

Padding: 1

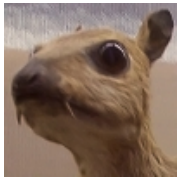
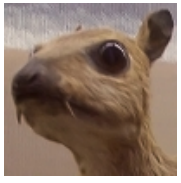
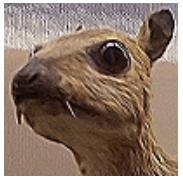
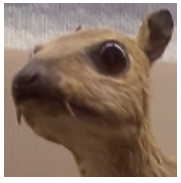
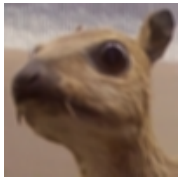
Processed

-3	-1	1	3	21
21	16	16	26	-23
-4	0	3	6	30
-3	3	7	11	25

Advanced Neural Networks: Feedforward Neural Networks (FFNN)

Convolutional Neural Network (CNN): Image processing (example of preprocessing)

An example from Wikipedia

Operation	Original	Kernel	Transformed
Edge detection		$\begin{bmatrix} -1 & -1 & -1 \\ -1 & 8 & -1 \\ -1 & -1 & -1 \end{bmatrix}$	
Sharpen		$\begin{bmatrix} 0 & -1 & 0 \\ -1 & 5 & -1 \\ 0 & -1 & 0 \end{bmatrix}$	
Box blur		$\frac{1}{9}\begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{bmatrix}$	

Advanced Neural Networks: Feedforward Neural Networks (FFNN)

Convolutional Neural Network (CNN): Limitations of the previous solution

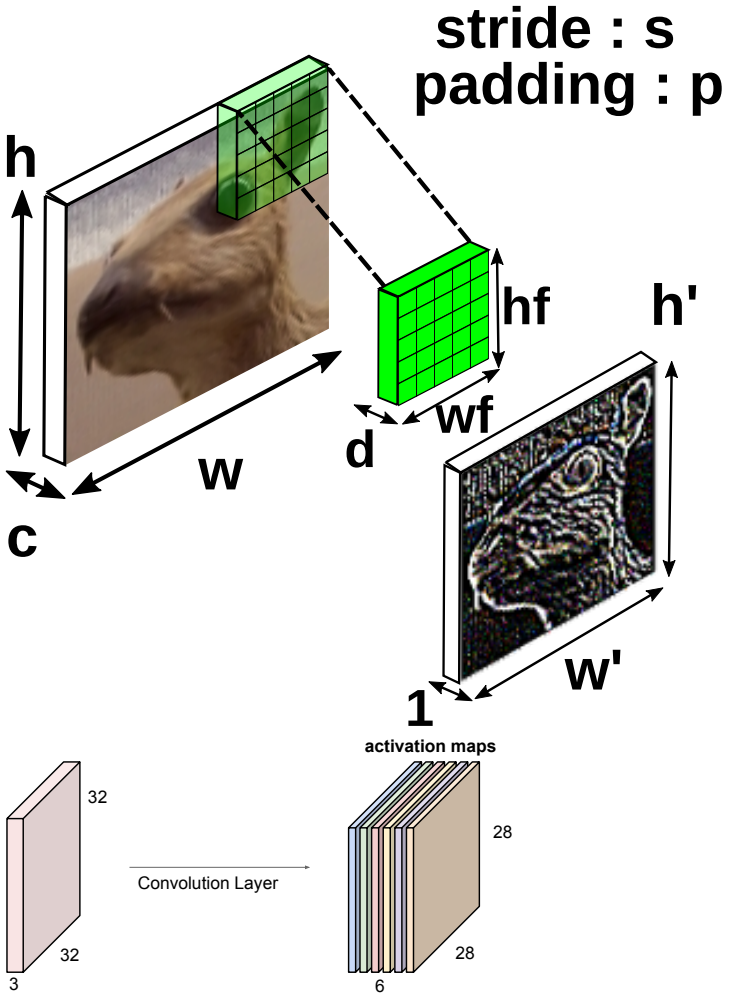
According to LeCun and his colleagues **[Lecun et al., 1998]**:

- When the size of the images is large, there will be a large number of parameters to train.
- To achieve this, a large dataset must be provided.
- The memory required to store the parameters will be very large.
- To train the model on images, preprocessing such as translations and distortions must be applied.
- Variations in images (such as the position of an object) can only be captured when multiple layers are used.

Advanced Neural Networks: Feedforward Neural Networks (FFNN)

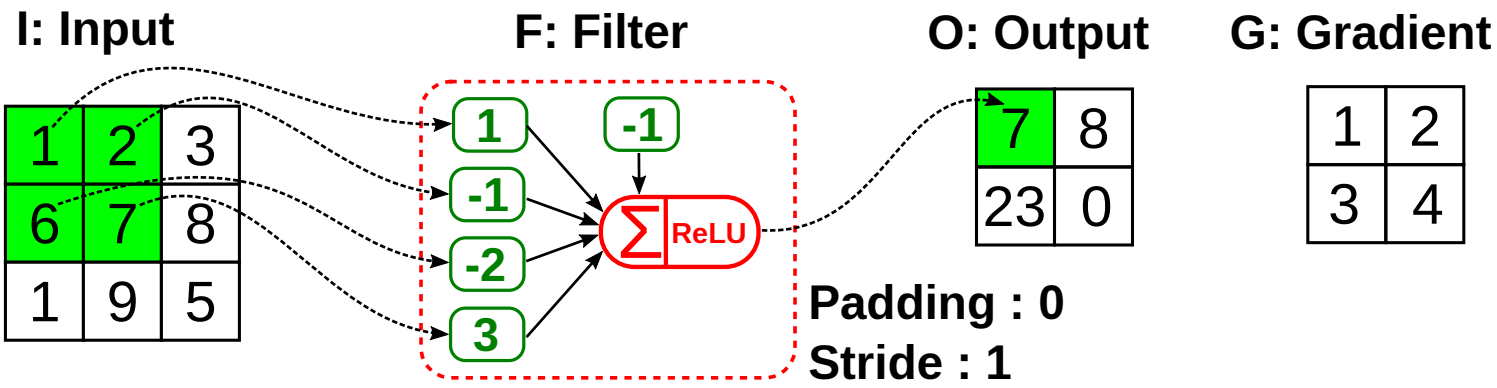
Convolutional Neural Network (CNN): Conv2D layer

- Preserve images' spatial structure.
- $w' = \frac{w - w_f + 2P}{S} + 1$, $h' = \frac{h - h_f + 2P}{S} + 1$
- A layer can have k filters/kernels.
- Number of parameters: $w_f * h_f * c * k$ plus k biases.
- Example, image: 32x32x3; kernel: 5x5; s: 1; p: 0; k: 6.
  Number of trainable parameters: 456



Advanced Neural Networks: Feedforward Neural Networks (FFNN)

Convolutional Neural Network (CNN): Conv2D layer (Example)



$$O_{11} = ReLU(\Sigma = b + F_{11}I_{11} + F_{12}I_{12} + F_{21}I_{21} + F_{22}I_{22})$$
$$O_{12} = ReLU(\Sigma = b + F_{11}I_{12} + F_{12}I_{13} + F_{21}I_{22} + F_{22}I_{23})$$
$$O_{21} = ReLU(\Sigma = b + F_{11}I_{21} + F_{12}I_{22} + F_{21}I_{31} + F_{22}I_{32})$$
$$O_{22} = ReLU(\Sigma = b + F_{11}I_{22} + F_{12}I_{23} + F_{21}I_{32} + F_{22}I_{33})$$

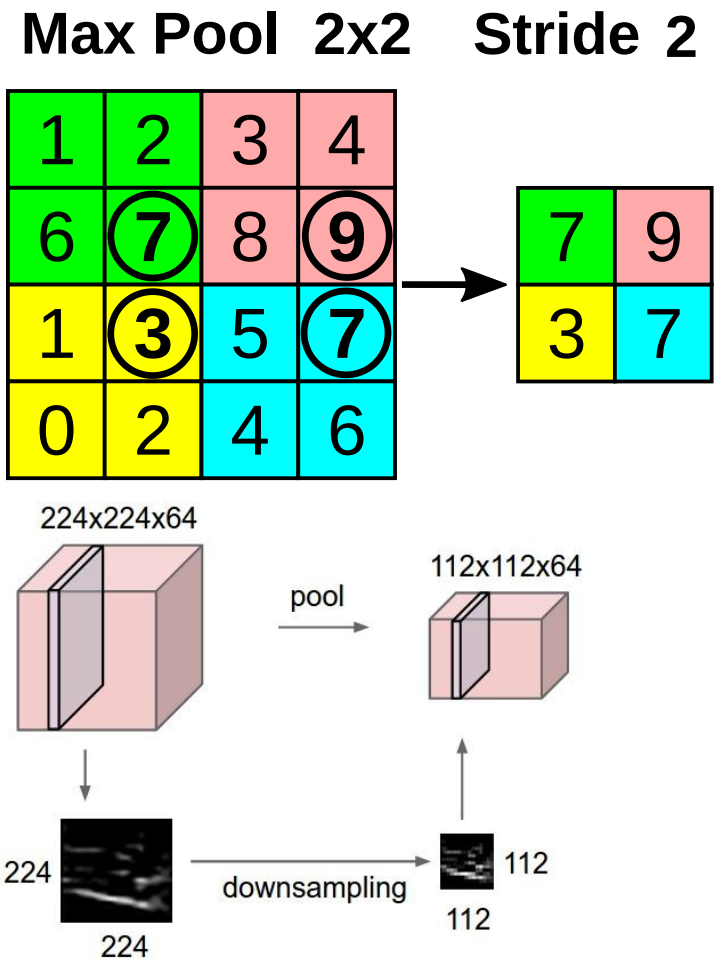
$$\frac{\partial J}{\partial I_{22}} = \underbrace{\frac{\partial J}{\partial O_{11}}}_{G_{11}=1} \underbrace{\frac{\partial ReLU}{\partial \sum}}_{1} \underbrace{\frac{\partial \sum}{\partial I_{22}}}_{F_{22}=3} + \underbrace{\frac{\partial J}{\partial O_{12}}}_{G_{12}=2} \underbrace{\frac{\partial ReLU}{\partial \sum}}_{1} \underbrace{\frac{\partial \sum}{\partial I_{22}}}_{F_{21}=-2} + \underbrace{\frac{\partial J}{\partial O_{21}}}_{G_{21}=3} \underbrace{\frac{\partial ReLU}{\partial \sum}}_{1} \underbrace{\frac{\partial \sum}{\partial I_{22}}}_{F_{12}=-1} + \underbrace{\frac{\partial J}{\partial O_{22}}}_{G_{22}=4} \underbrace{\frac{\partial ReLU}{\partial \sum}}_{0} \underbrace{\frac{\partial \sum}{\partial I_{22}}}_{F_{11}=1}$$

$$\frac{\partial J}{\partial I_{12}} = \underbrace{\frac{\partial J}{\partial O_{11}}}_{G_{11}=1} \underbrace{\frac{\partial ReLU}{\partial \sum}}_{1} \underbrace{\frac{\partial \sum}{\partial I_{12}}}_{F_{12}=-1} + \underbrace{\frac{\partial J}{\partial O_{12}}}_{G_{12}=2} \underbrace{\frac{\partial ReLU}{\partial \sum}}_{1} \underbrace{\frac{\partial \sum}{\partial I_{12}}}_{F_{11}=1}$$

Advanced Neural Networks: Feedforward Neural Networks (FFNN)

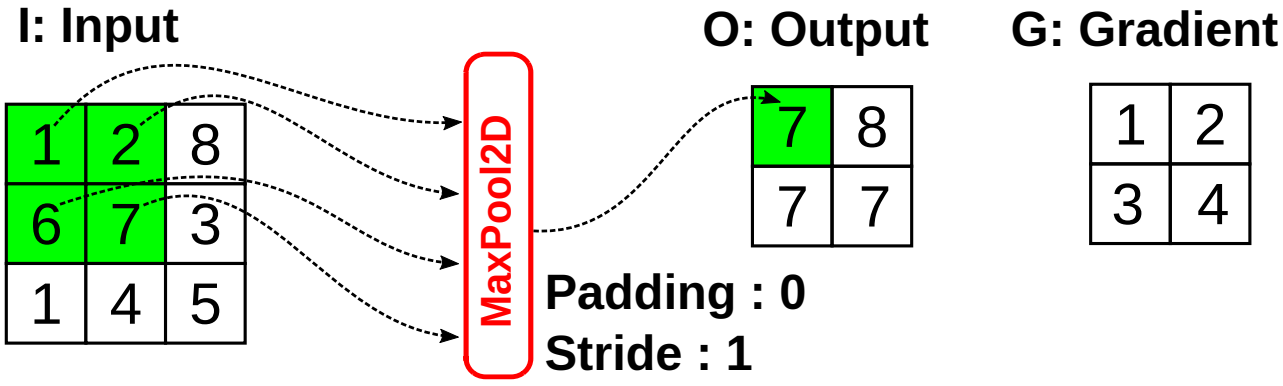
Convolutional Neural Network (CNN): Pooling

- Make the representation smaller and more manageable.
- $w' = \frac{w - w_f + 2P}{S} + 1, h' = \frac{h - h_f + 2P}{S} + 1$
- No parameters.
- **Max Pool**: The gradient is only passed to the winning cell. If there are multiple max values, choose one (usually the first).
- **Average Pool**: The average gradient is passed to participating cells. Each cell will have a gradient $\frac{\text{gradient}}{w_f * h_f}$.



Advanced Neural Networks: Feedforward Neural Networks (FFNN)

Convolutional Neural Network (CNN): MaxPool2D layer (Example)



$$O_{11} = Max(I_{11} + I_{12} + I_{21} + I_{22}) = I_{22}$$
$$O_{12} = Max(I_{12} + I_{13} + I_{22} + I_{23}) = I_{23}$$
$$O_{21} = Max(I_{21} + I_{22} + I_{31} + I_{32}) = I_{22}$$
$$O_{22} = Max(I_{22} + I_{23} + I_{32} + I_{33}) = I_{22}$$

$$\frac{\partial J}{\partial I_{22}} = \underbrace{\frac{\partial J}{\partial O_{11}}}_{G_{11}=1} \underbrace{\frac{\partial Max}{\partial I_{22}}}_{1} + \underbrace{\frac{\partial J}{\partial O_{12}}}_{G_{12}=2} \underbrace{\frac{\partial Max}{\partial I_{22}}}_{0} + \underbrace{\frac{\partial J}{\partial O_{21}}}_{G_{21}=3} \underbrace{\frac{\partial Max}{\partial I_{22}}}_{1} + \underbrace{\frac{\partial J}{\partial O_{22}}}_{G_{22}=4} \underbrace{\frac{\partial Max}{\partial I_{22}}}_{1}$$

$$\frac{\partial J}{\partial I_{12}} = \underbrace{\frac{\partial J}{\partial O_{11}}}_{G_{11}=1} \underbrace{\frac{\partial Max}{\partial I_{12}}}_{0} + \underbrace{\frac{\partial J}{\partial O_{12}}}_{G_{12}=2} \underbrace{\frac{\partial Max}{\partial I_{12}}}_{0}$$

Advanced Neural Networks: Feedforward Neural Networks (FFNN)

Convolutional Neural Network (CNN): Some humor

Advanced Neural Networks: Feedforward Neural Networks (FFNN)

Regularization: Droupout

- When training large neural networks on a small dataset, overfitting can occur.
- One solution is to reduce the size of the network.
- Another is to temporarily deactivate connections in a random manner.
- This technique is called **dropout**.
- The dropout layer takes a dropout rate as a parameter.
- This layer deactivates some outputs (considers them as 0) during training (not during inference).

Advanced Neural Networks: Feedforward Neural Networks (FFNN)

Regularization: Some humor

If Thanos were a Data Scientist

Section 3

Recurrent Neural Networks (RNN)

Advanced Neural Networks

Recurrent Neural Networks (RNN)

Definition

A ”Recurrent Neural Network” is an architecture of Neural Networks. In this one, there is a ”feed” back from the outputs of the neurons to the inputs throughout the network. **[Sazlı, 2006]**

In other word, there is a temporal phenomena treated in the problem in question; current output depends on the past one.

Example

- Predicting future weather based on some features, plus the current one

Advanced Neural Networks: Recurrent Neural Networks (RNN)

Architecture (RNN)

- **Elman network**

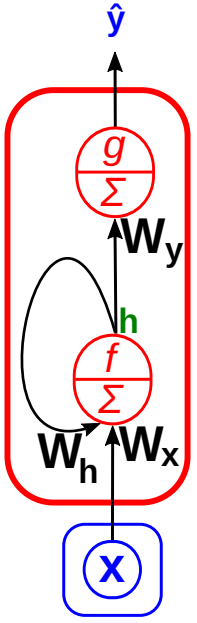
$$h_t = f(w_x x_t + w_h h_{t-1} + b_h)$$
$$\hat{y}_t = g(w_y h_t + b_y)$$

- **Jordan network**

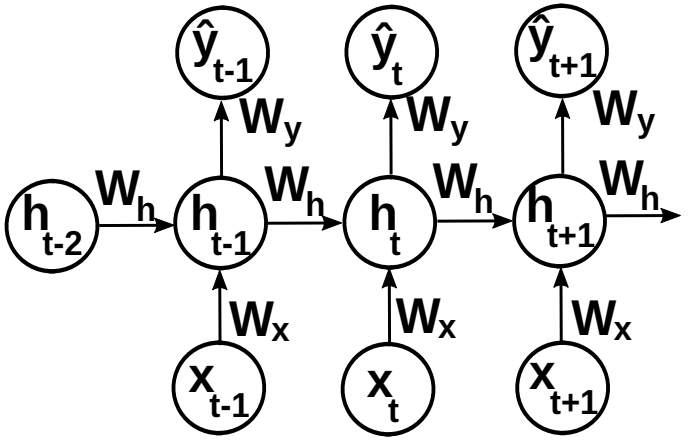
$$h_t = f(w_x x_t + w_h \hat{y}_{t-1} + b_h)$$
$$\hat{y}_t = g(w_y h_t + b_y)$$

RNN

$$h_t = f(W_x x_t + W_h h_{t-1} b_h)$$
$$y_t = g(W_y h_t + b_y)$$



Unfolded network



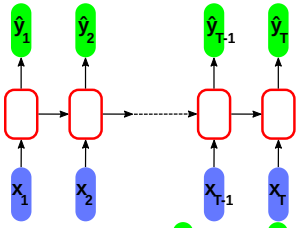
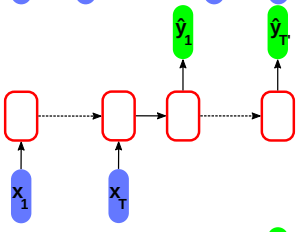
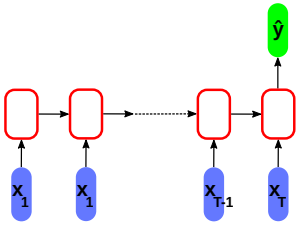
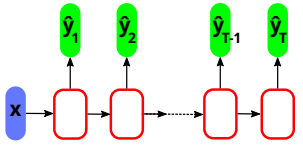
Advanced Neural Networks: Recurrent Neural Networks (RNN)

Architecture (RNN): Backpropagation

- Define the cost function for each output.
- Use backpropagation through time **[Werbos, 1990]**
  - Unroll the recurrent network over time.
  - The network will be similar to a feed-forward one.
  - Accumulate gradients starting from the last state.
  - Update parameters when reaching the first state.

Advanced Neural Networks: Recurrent Neural Networks (RNN)

Architecture (RNN): Applications

Type	Illustration	Example
Many to many		Named entity detection
Many to many (Seq2seq)		Machine translation
Many to one		Sentiment classification
One to many		Image caption generation

Advanced Neural Networks: Recurrent Neural Networks (RNN)

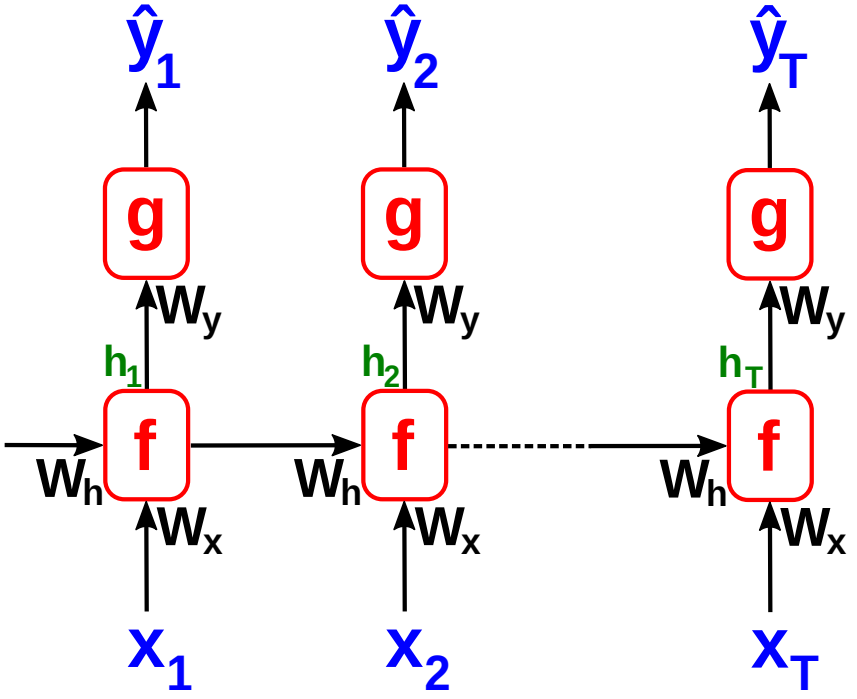
Architecture (RNN): Applications (direct many to many)

h_0 is a predefined victor

$$h_t = f(x_t, h_{t-1}, W_x, W_h)$$

$$\hat{y}_t = g(h_t, W_y)$$

$$J(\hat{y}, y) = \frac{1}{T} \sum_{t=1}^{T} j(\hat{y}_t, y_t)$$



Advanced Neural Networks: Recurrent Neural Networks (RNN)

Architecture (RNN): Applications (direct many to many: Back-propagation)

$$\frac{\partial J}{\partial W_y} = \frac{1}{T}\sum_{t=1}^{T}\frac{\partial j(\hat{y}_t, y_t)}{\partial W_y} = \frac{1}{T}\sum_{t=1}^{T}\frac{\partial j(\hat{y}_t, y_t)}{\partial \hat{y}_t}\frac{\partial g(h_t, W_y)}{\partial W_y}$$

$$\frac{\partial J}{\partial W_h} = \frac{1}{T}\sum_{t=1}^{T}\frac{\partial j(\hat{y}_t, y_t)}{\partial W_h} = \frac{1}{T}\sum_{t=1}^{T}\frac{\partial j(\hat{y}_t, y_t)}{\partial \hat{y}_t}\frac{\partial g(h_t, W_y)}{\partial h_t}\frac{\partial h_t}{\partial W_h}$$

$$\frac{\partial h_t}{\partial W_h} = \frac{\partial f(x_t, h_{t-1}, W_x, W_h)}{\partial W_h} + \frac{\partial f(x_t, h_{t-1}, W_x, W_h)}{\partial h_{t-1}}\frac{\partial h_{t-1}}{\partial W_h}$$

$$\frac{\partial J}{\partial W_x} = \frac{1}{T}\sum_{t=1}^{T}\frac{\partial j(\hat{y}_t, y_t)}{\partial W_x} = \frac{1}{T}\sum_{t=1}^{T}\frac{\partial j(\hat{y}_t, y_t)}{\partial \hat{y}_t}\frac{\partial g(h_t, W_y)}{\partial h_t}\frac{\partial h_t}{\partial W_x}$$

$$\frac{\partial h_t}{\partial W_x} = \frac{\partial f(x_t, h_{t-1}, W_x, W_h)}{\partial W_x} + \frac{\partial f(x_t, h_{t-1}, W_x, W_h)}{\partial h_{t-1}}\frac{\partial h_{t-1}}{\partial W_x}$$

Advanced Neural Networks: Recurrent Neural Networks (RNN)

Architecture (RNN): Applications (direct many to many: Problem)

$\frac{\partial h_t}{\partial W_h}$ can be simplified:

$$\frac{\partial h_t}{\partial W_h} = \frac{\partial f(x_t, h_{t-1}, W_x, W_h)}{\partial W_h} + \sum_{i=1}^{t-1} \left(\prod_{j=i+1}^{t} \frac{\partial f(x_j, h_{j-1}, W_x, W_h)}{\partial h_{j-1}} \right) \frac{\partial f(x_i, h_{i-1}, W_x, W_h)}{\partial W_h}$$

- Can result in ***vanishing gradients*** (e.g. $f = \sigma(\sum)$)
- Also, ***exploding gradients*** (e.g. $f = ReLU(\sum)$)
- Possible solution: Truncating time steps **[Jaeger, 2002]**

Advanced Neural Networks: Recurrent Neural Networks (RNN)

Architecture (RNN): Applications (Seq2seq)

Encoder

h_0 is a predefined victor

$$h_t^e = f^e(x_t, h_{t-1}^e, W_x^e, W_h^e)$$

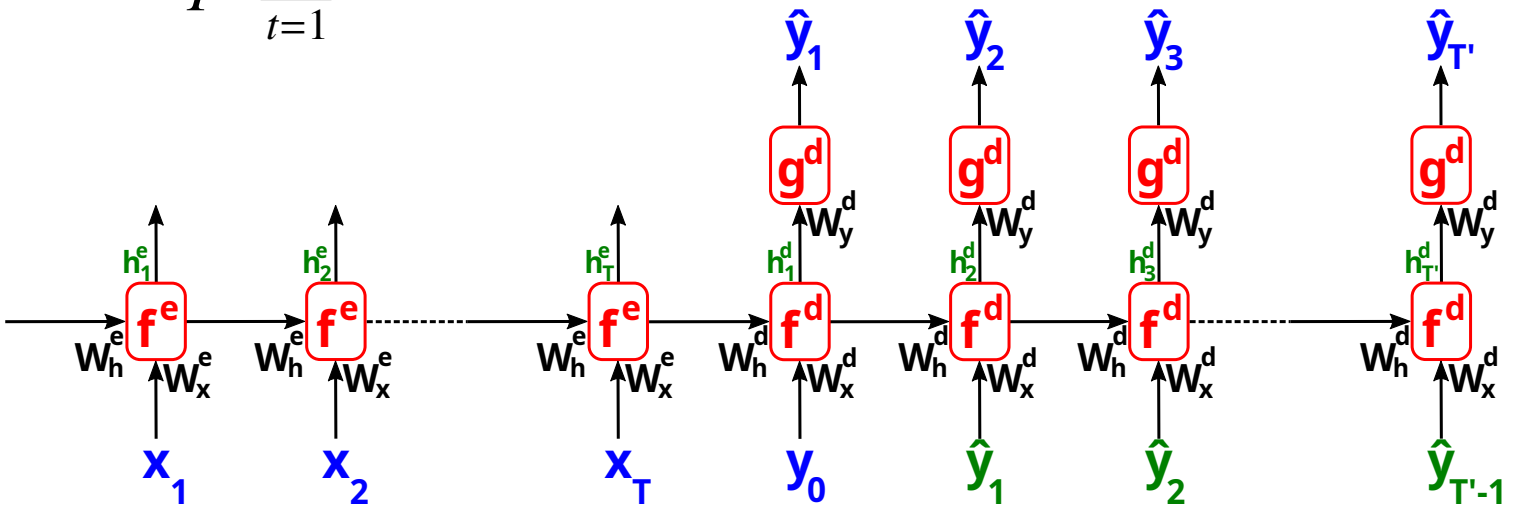
$$J(\hat{y}, y) = \frac{1}{T'} \sum_{t=1}^{T'} j(\hat{y}_t, y_t)$$

Decoder

$h_0^d = h_T^e$, y_0 is a predefined victor

$$h_t^d = f^d(\hat{y}_{t-1}, h_{t-1}^d, W_x^d, W_h^d)$$

$$\hat{y}_t = g^d(h_{t-1}^d, W_y^d)$$



Advanced Neural Networks: Recurrent Neural Networks (RNN)

Architecture (RNN): Applications (Seq2seq: Back-propagation)

- Decoder cell is updated as direct Many2Many, replacing x_t by $\hat{y}_{t-1}$
- Encoder cell is updated as direct Many2Many, but without direct output

TODO: Revise (my brain is killing me)

$$\frac{\partial J}{\partial W_h^e} = \frac{\partial J}{\partial h_T^e}\frac{\partial h_T^e}{\partial W_h^e} \quad \frac{\partial J}{\partial W_x^e} = \frac{\partial J}{\partial h_T^e}\frac{\partial h_T^e}{\partial W_x^e}$$

$$\frac{\partial J}{\partial h_T^e} = \frac{\partial J}{\partial h_0^d} = \frac{1}{T'}\sum_{t=1}^{T'}\frac{\partial j(\hat{y}_t, y_t)}{\partial h_0^d} = \frac{1}{T'}\sum_{t=1}^{T'}\frac{\partial j(\hat{y}_t, y_t)}{\partial \hat{y}_t}\frac{\partial g(h_t^d, W_y^d)}{\partial h_t^d}\frac{\partial h_t^d}{\partial h_0^d}$$

$$\frac{\partial h_t^d}{\partial h_0^d} = \frac{\partial f^d(\hat{y}_{t-1}, h_{t-1}^d, W_x^d, W_h^d)}{\partial h_{t-1}^d}\frac{\partial h_{t-1}^d}{\partial h_0^d} = \prod_{i=1}^{t}\frac{\partial f^d(\hat{y}_{i-1}, h_{i-1}^d, W_x^d, W_h^d)}{\partial h_{i-1}^d}$$

Advanced Neural Networks: Recurrent Neural Networks (RNN)

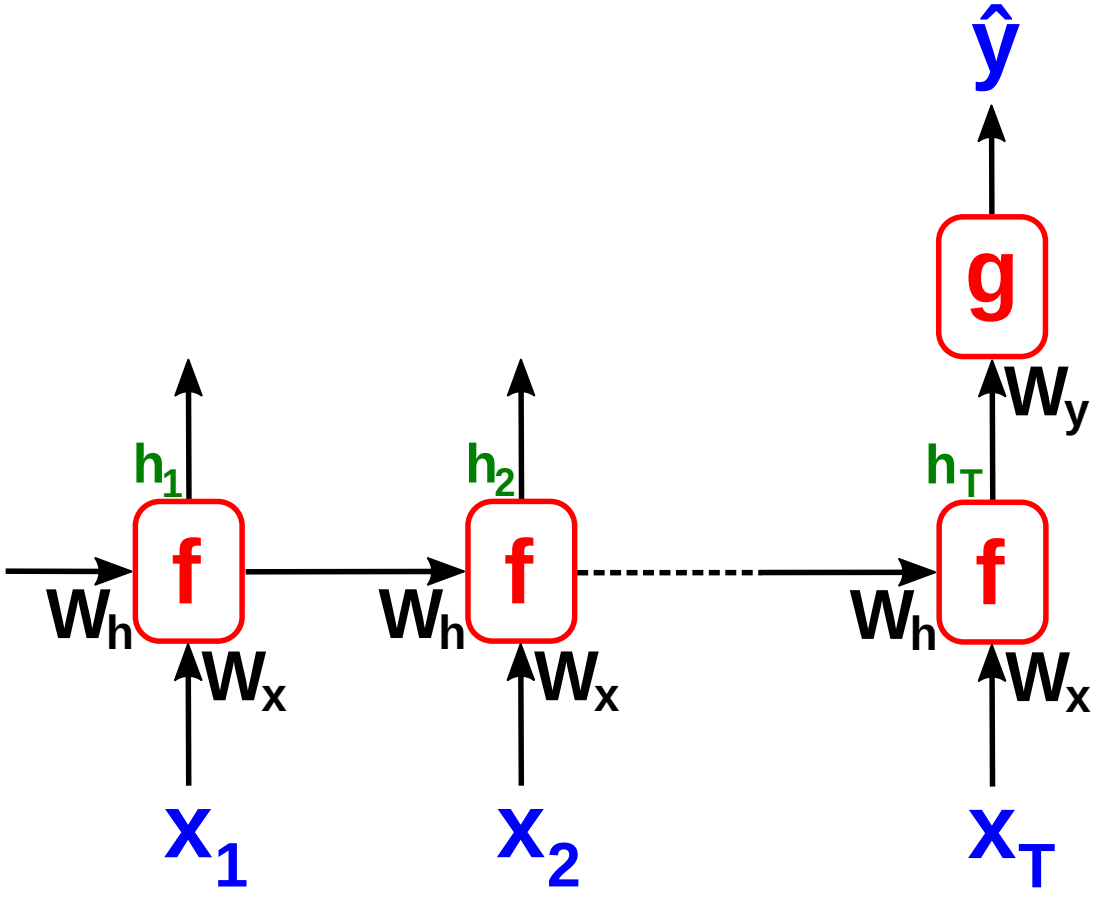
Architecture (RNN): Applications (many to one)

h_0 is a predefined victor

$$h_t = f(x_t, h_{t-1}, W_x, W_h)$$

$$\hat{y} = g(h_T, W_y)$$

$$J(\hat{y}, y) = j(\hat{y}, y)$$



Advanced Neural Networks: Recurrent Neural Networks (RNN)

Architecture (RNN): Applications (many to one: Back-propagation)

$$\frac{\partial J}{\partial W_y} = \frac{\partial j(\hat{y}, y)}{\partial W_y} = \frac{\partial j(\hat{y}, y)}{\partial \hat{y}} \frac{\partial g(h_T, W_y)}{\partial W_y}$$

$$\frac{\partial J}{\partial W_h} = \frac{\partial j(\hat{y}, y)}{\partial W_h} = \frac{\partial j(\hat{y}, y)}{\partial \hat{y}} \frac{\partial g(h_T, W_y)}{\partial h_T} \frac{\partial h_T}{\partial W_h}$$

$$\frac{\partial h_t}{\partial W_h} = \frac{\partial f(x_t, h_{t-1}, W_x, W_h)}{\partial W_h} + \frac{\partial f(x_t, h_{t-1}, W_x, W_h)}{\partial h_{t-1}} \frac{\partial h_{t-1}}{\partial W_h}$$

$$\frac{\partial J}{\partial W_x} = \frac{\partial j(\hat{y}, y)}{\partial W_x} = \frac{\partial j(\hat{y}, y)}{\partial \hat{y}} \frac{\partial g(h_T, W_y)}{\partial h_T} \frac{\partial h_T}{\partial W_x}$$

$$\frac{\partial h_t}{\partial W_x} = \frac{\partial f(x_t, h_{t-1}, W_x, W_h)}{\partial W_x} + \frac{\partial f(x_t, h_{t-1}, W_x, W_h)}{\partial h_{t-1}} \frac{\partial h_{t-1}}{\partial W_x}$$

Advanced Neural Networks: Recurrent Neural Networks (RNN)

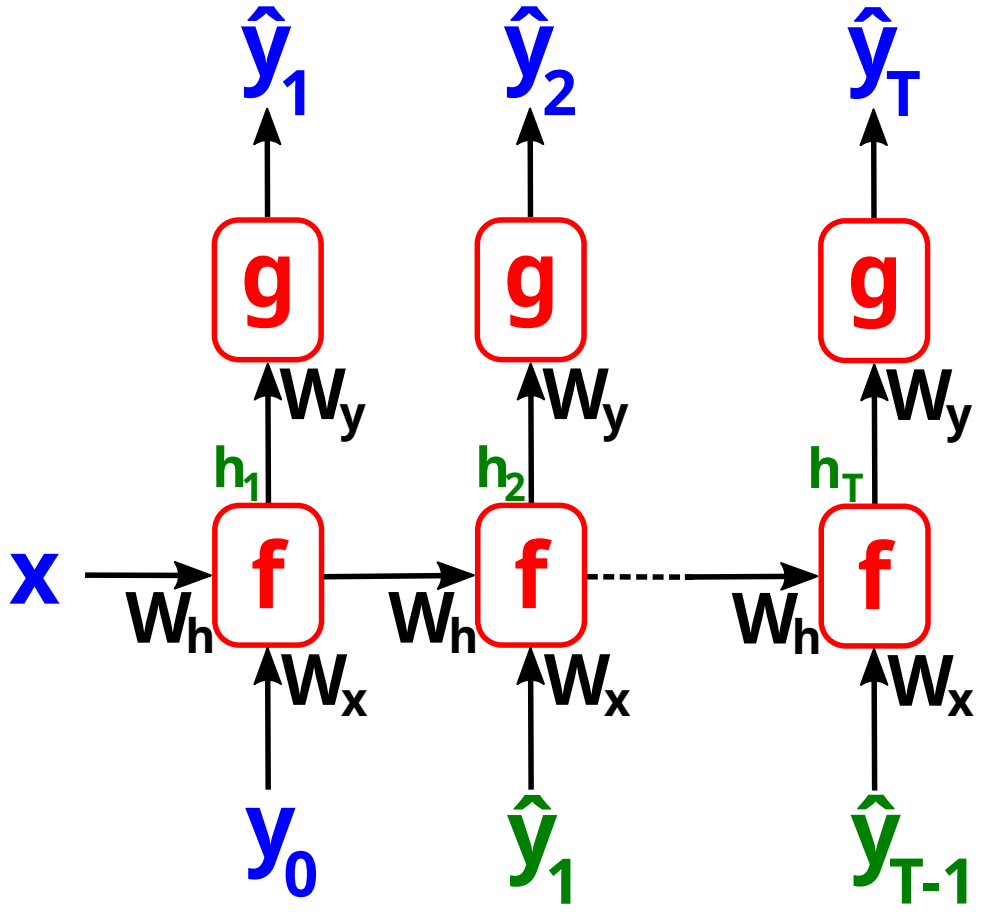
Architecture (RNN): Applications (one to many)

$$h_1 = f(y_0, x, W_x, W_h)$$

$$h_t = f(\hat{y}_{t-1}, h_{t-1}, W_y, W_h)$$

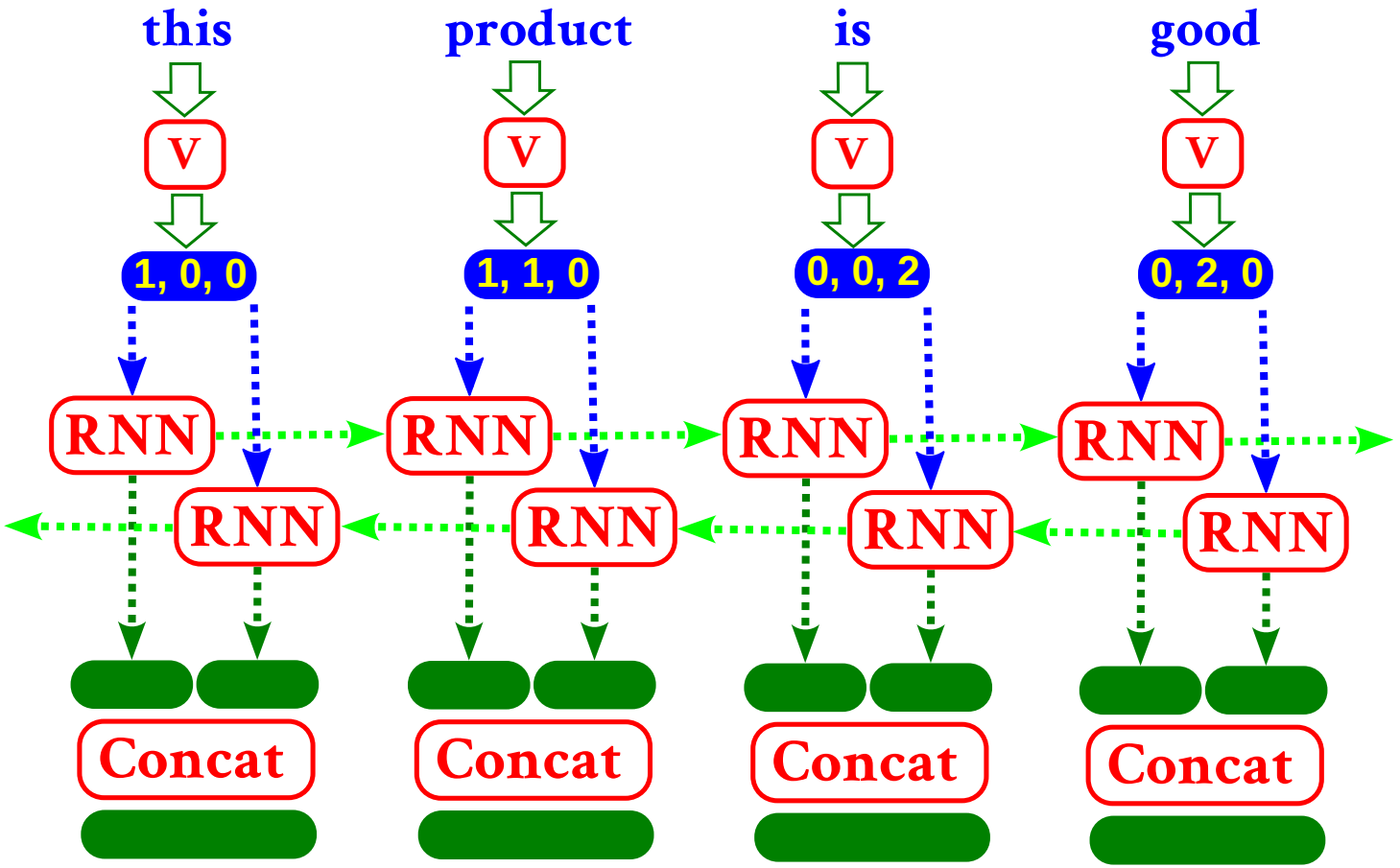
$$\hat{y}_t = g(h_t, W_y)$$

$$J(\hat{y}, y) = \frac{1}{T} \sum_{t=1}^{T} j(\hat{y}_t, y_t)$$



Advanced Neural Networks: Recurrent Neural Networks (RNN)

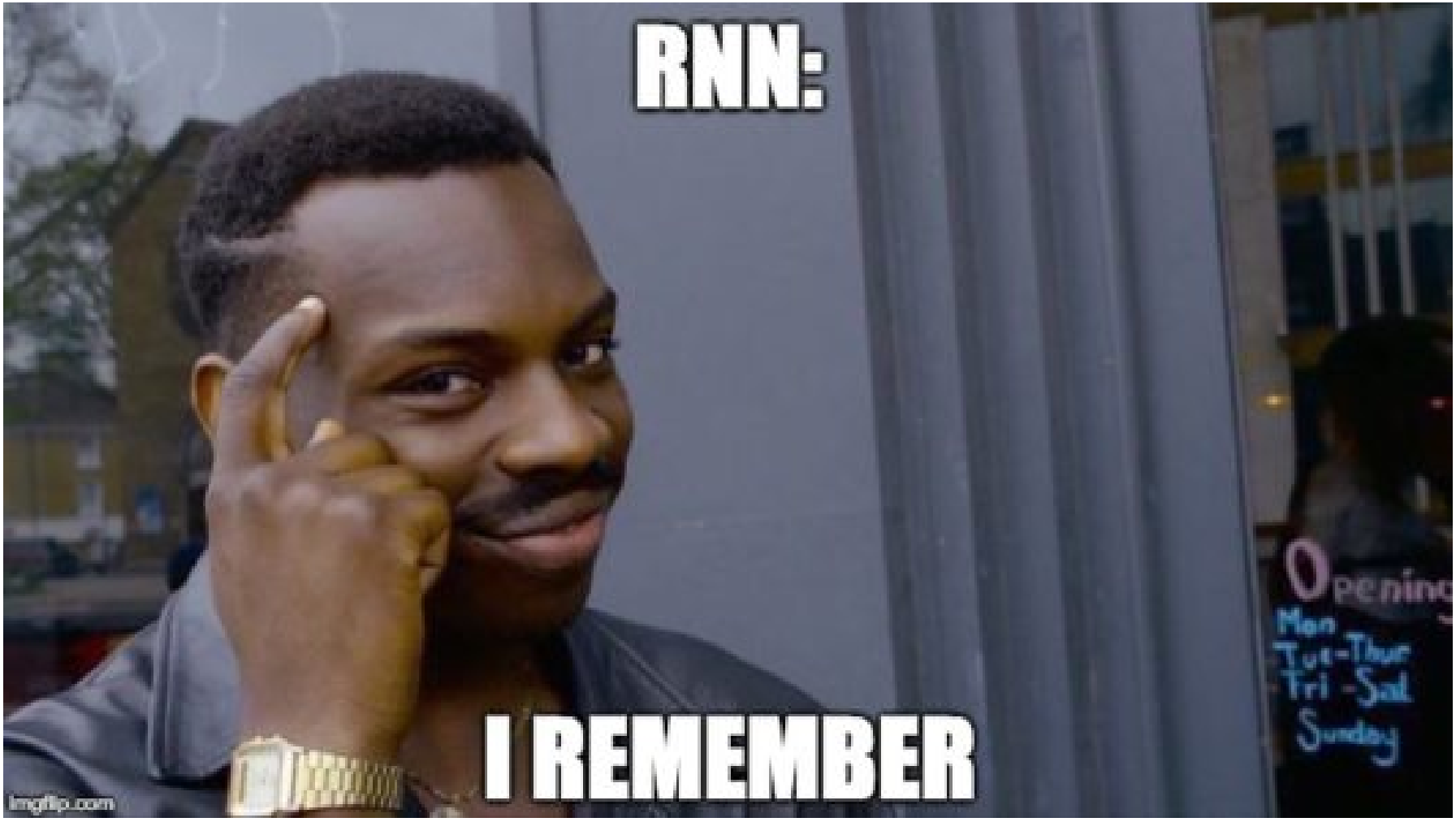
Architecture (RNN): Bidirectional RNN



V Words' vectorization function (embedding)

Advanced Neural Networks: Recurrent Neural Networks (RNN)

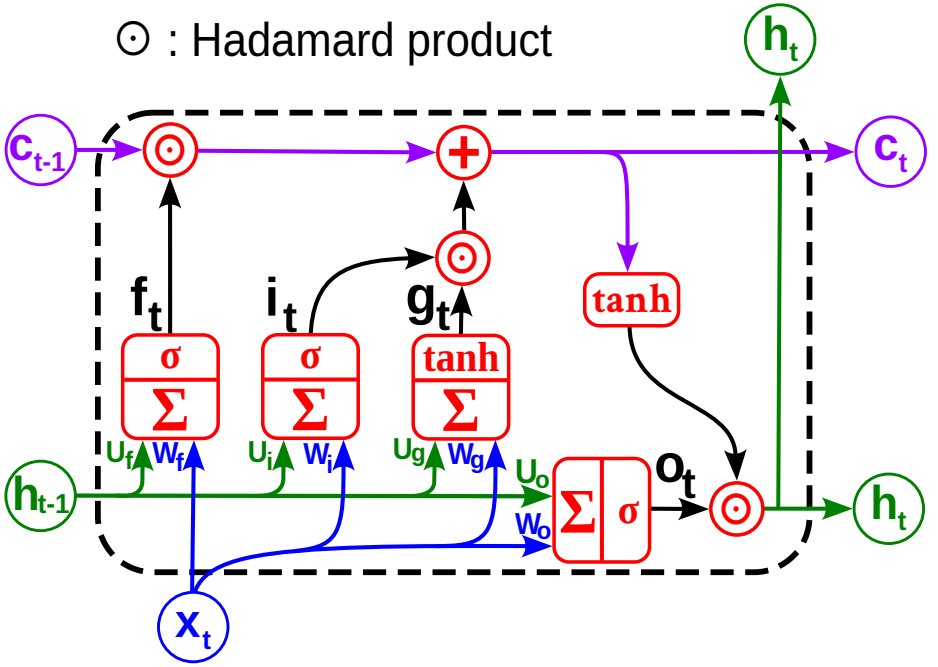
Architecture (RNN): Some humor



Advanced Neural Networks: Recurrent Neural Networks (RNN)

Long Short-Term Memory (LSTM): Architecture

- i: **input gate**; How much information will be added to the cell's intern state?
- f: **Forget gate**; Must the past state be forgotten?
- o: **Output gate** ; Combining the cell's intern and current states



- g: **Input node**; Will the state be increased or decreased? (mostly considered to be a part of input gate)

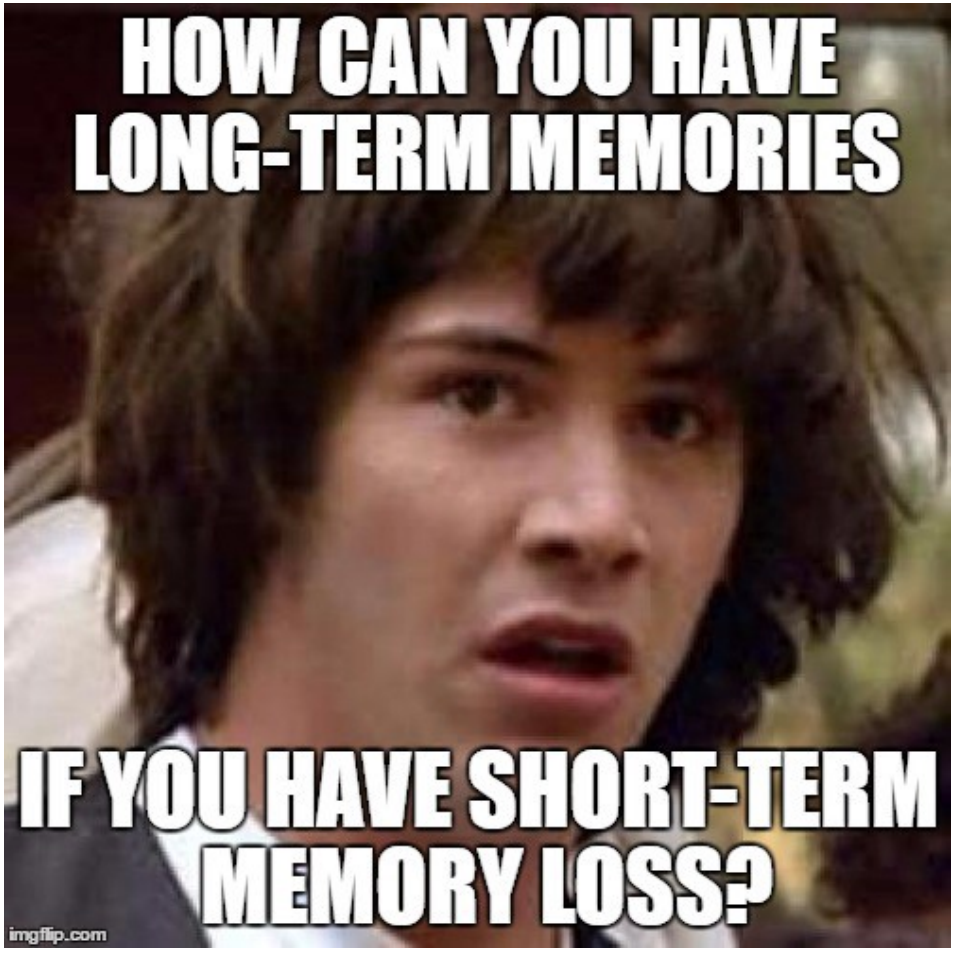
Advanced Neural Networks: Recurrent Neural Networks (RNN)

Long Short-Term Memory (LSTM): Equations

$$f_t = \sigma(W_f X_t + U_f h_{t-1} + b_f)$$
$$i_t = \sigma(W_i X_t + U_i h_{t-1} + b_i)$$
$$g_t = \tanh(W_g X_t + U_g h_{t-1} + b_g)$$
$$o_t = \tanh(W_o X_t + U_o h_{t-1} + b_o)$$
$$c_t = f_t \circ c_{t-1} \oplus i_t \circ g_t$$
$$h_t = o_t + \tanh(c_t)$$

Advanced Neural Networks: Recurrent Neural Networks (RNN)

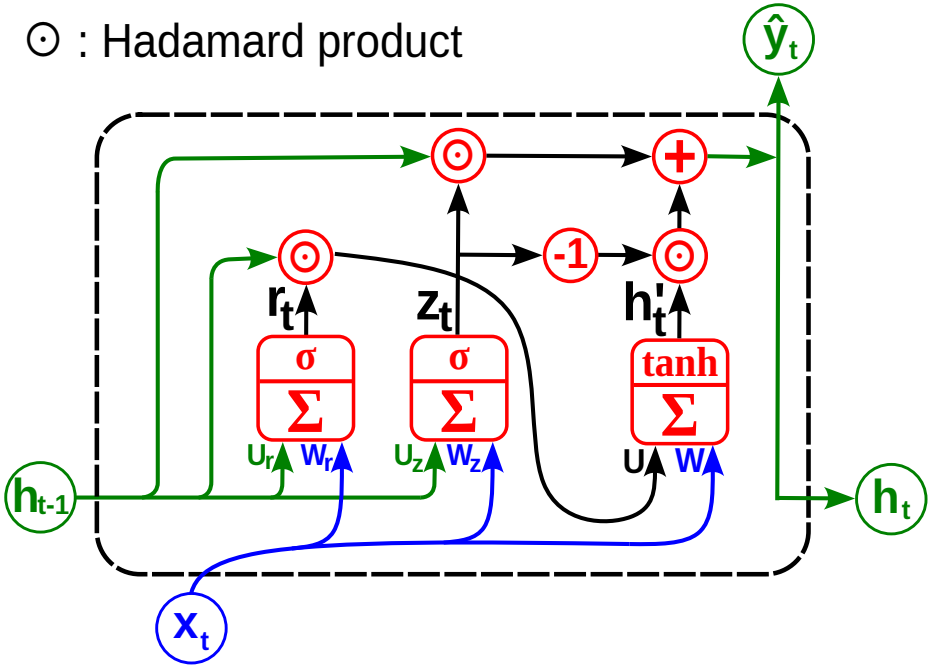
Long Short-Term Memory (LSTM): Some humor



Advanced Neural Networks: Recurrent Neural Networks (RNN)

Gated Recurrent Unit (GRU): Architecture

- z: **Update gate**; Merges LSTM's input and forget gates.
- r: **Reset gate**; How much update from the past state?
- h': **Candidate hidden state**; Current state.



Advanced Neural Networks: Recurrent Neural Networks (RNN)

Gated Recurrent Unit (GRU): Equations

$$z_t = \sigma(W_z X_t + U_z h_{t-1} + b_z)$$
$$r_t = \sigma(W_r X_t + U_r h_{t-1} + b_r)$$
$$h'_t = \tanh(W X_t + U(h_{t-1} \circ r_t) + b)$$
$$h_t = z_t \circ h_{t-1} \oplus (1 - z_t) \circ h'_{t-1}$$

Advanced Neural Networks: Recurrent Neural Networks (RNN)

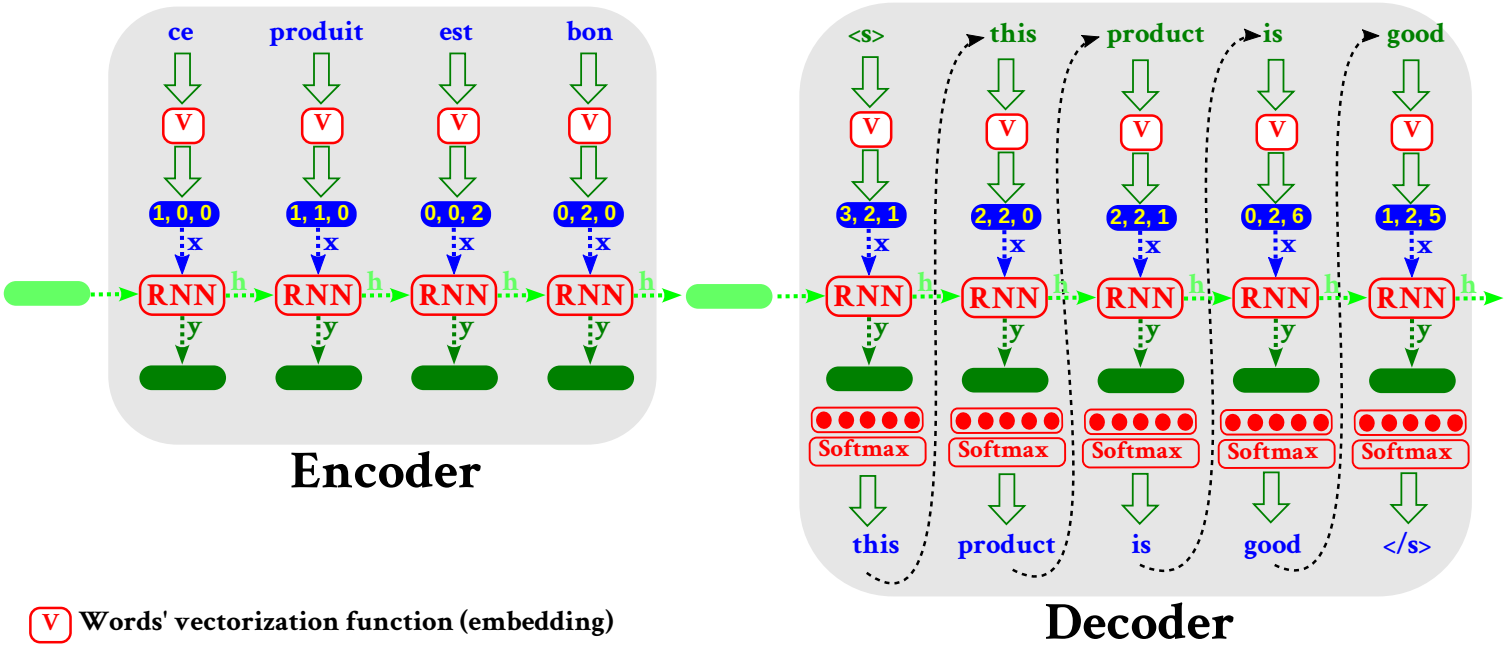
Gated Recurrent Unit (GRU): Some humor

Section 4

Attention

Advanced Neural Networks

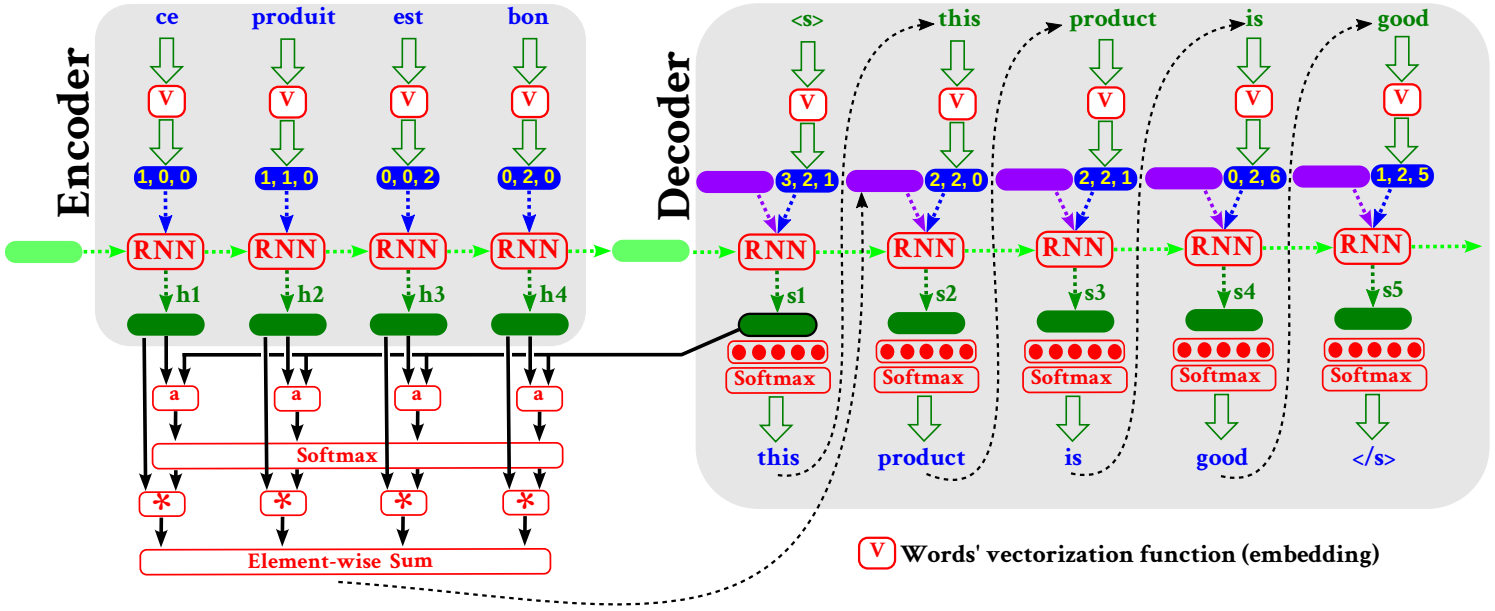
Attention: Motivation



- Model: Seq2Seq (Encoder-Decoder)
- Long-term dependencies are not considered.
- The generation of target words depends only on previously generated words and the last words of the original text.

Advanced Neural Networks: Attention

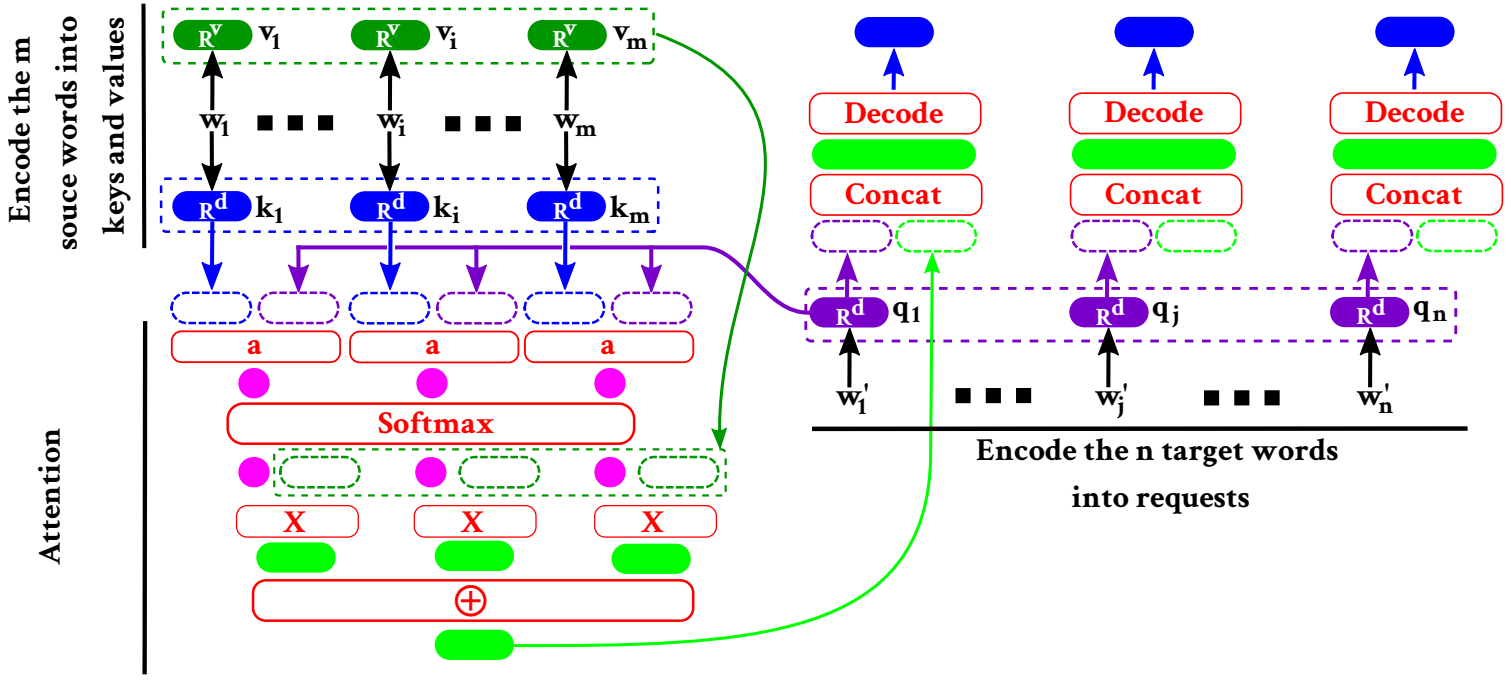
Attention mechanism



- Keep T hidden states from the encoder: h_i
- For each s_{t-1}, calculate its alignment with the hidden states.
  $e_{t,i} = a(s_{t-1}, h_i)$
- Calculate the weights of the hidden states: $\alpha_{t,i} = \text{softmax}(e_{t,i})$
- Calculate the state vector $c_t = \sum_{i=1}^{T} \alpha_{t,i} h_i$

Advanced Neural Networks: Attention

Attention mechanism: Formalism (1)



- Keys (k_i): m states which are used to estimate values' weights
- Values (v_i): m states used to construct the context
- Queries (q_j): current representation

Advanced Neural Networks: Attention

Attention mechanism: Formalism (2)

- Let $w_1 \cdots w_m$ a source sequence
  - $k_i = Embedding_k(w_i)$ a vector of d elements
  - $v_i = Embedding_v(w_i)$ a vector of v elements
- Let w'_j a current target word
  - $q_j = Embedding_q(w'_j)$ a vector of d elements
- Calculate a similarity between each key k_i and our current target word

$$e_i = a(q_j, k_i)$$

- Calculate the percentage similarity (softmax can be masked)

$$\alpha_i = softmax(e_i) = \frac{exp(e_i)}{\sum_k exp(e_k)}$$

- The attention is a vector formed by cumulating percentages of each value vector

$$attention(q, K, V) = \sum_{i=1}^{m} \alpha_i v_i$$

Advanced Neural Networks: Attention

Attention mechanism: Attention functions (non parametric)

$$Q \in \mathbb{R}^{n \times d},\ K \in \mathbb{R}^{m \times d},\ a(Q,K) \in \mathbb{R}^{n \times m},\ V \in \mathbb{R}^{m \times v}$$

Dot product (**tf.keras.layers.Attention**)

$$a(Q,K) = Q \cdot K^\top$$

Scaled dot product

$$a(Q,K) = \frac{Q \cdot K^\top}{\sqrt{d}}$$

Cosine similarity

$$a(Q,K) = \frac{Q \cdot K^\top}{||Q||\,||K||}$$

Advanced Neural Networks: Attention

Attention mechanism: Attention functions (parametric)

$$Q \in \mathbb{R}^{n \times d},\ K \in \mathbb{R}^{m \times d},\ a(Q,K) \in \mathbb{R}^{n \times m},\ V \in \mathbb{R}^{m \times v}$$

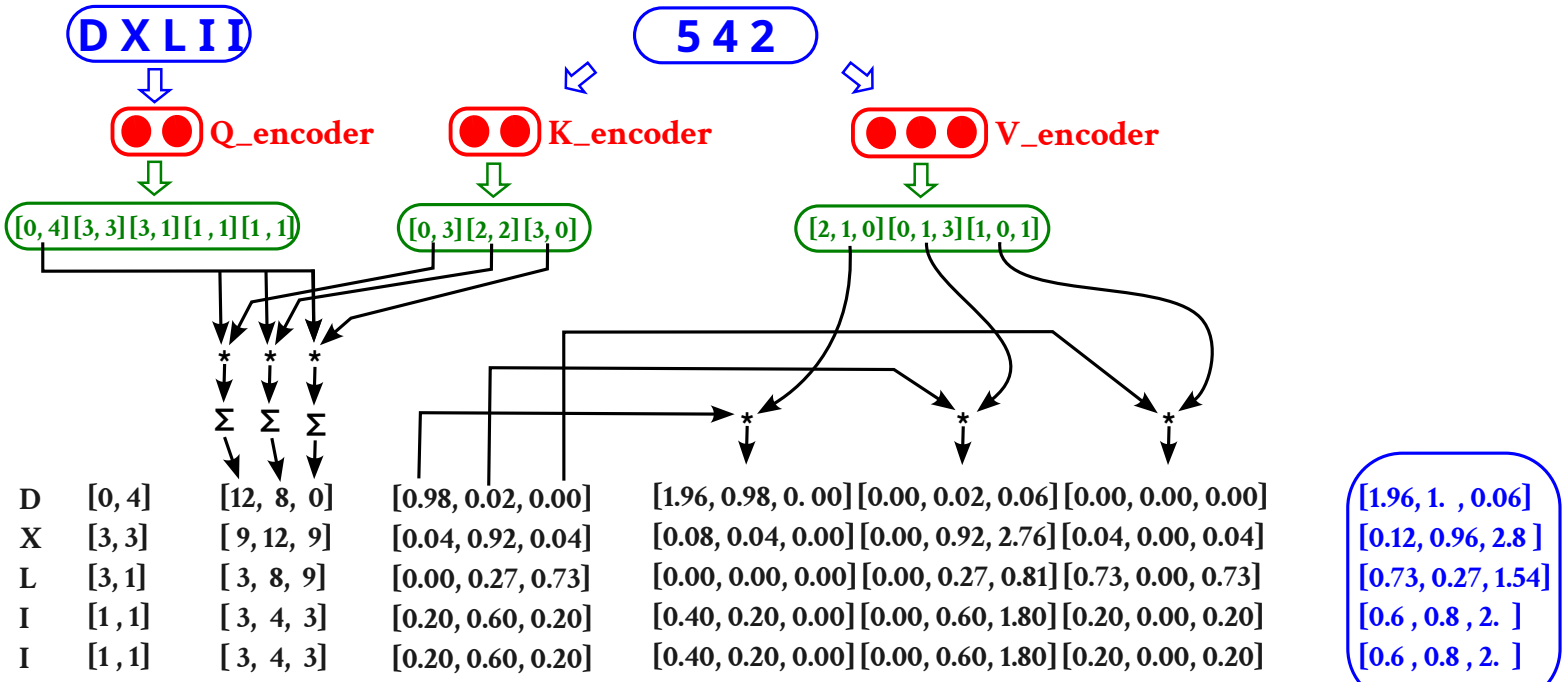
Additive attention (**tf.keras.layers.AdditiveAttention**)
Bahdanau Attention

$$a(Q,K) = W_v^\top \cdot \tanh(W_q Q + W_k K)$$

Advanced Neural Networks: Attention

Attention mechanism: Numerical example

Arabic numeral into Roman numeral transformation; 542 = DXLII.
We want to encode each Roman digit according to their attention with the Arabic digits



$e = Q \cdot K^T$
Attention function

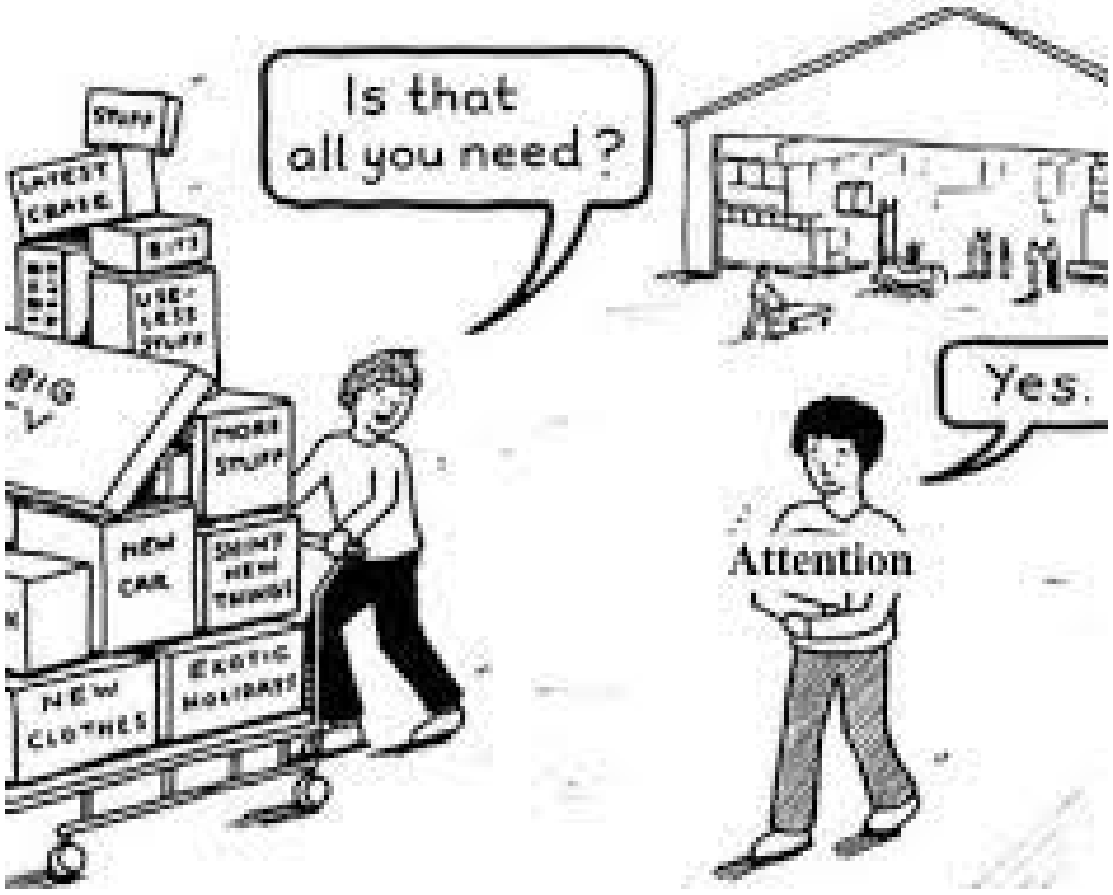
$\alpha = Softmax(e)$
Attention percentage

$V'_i = V_i * \alpha_i$
Multiply Each value vector by the equivalent percentage

$\sum V'_i$
Element-wise Sum over weighted value vectors

Advanced Neural Networks: Attention

Attention mechanism: Some humor



Advanced Neural Networks: Attention

Multi-Head Attention

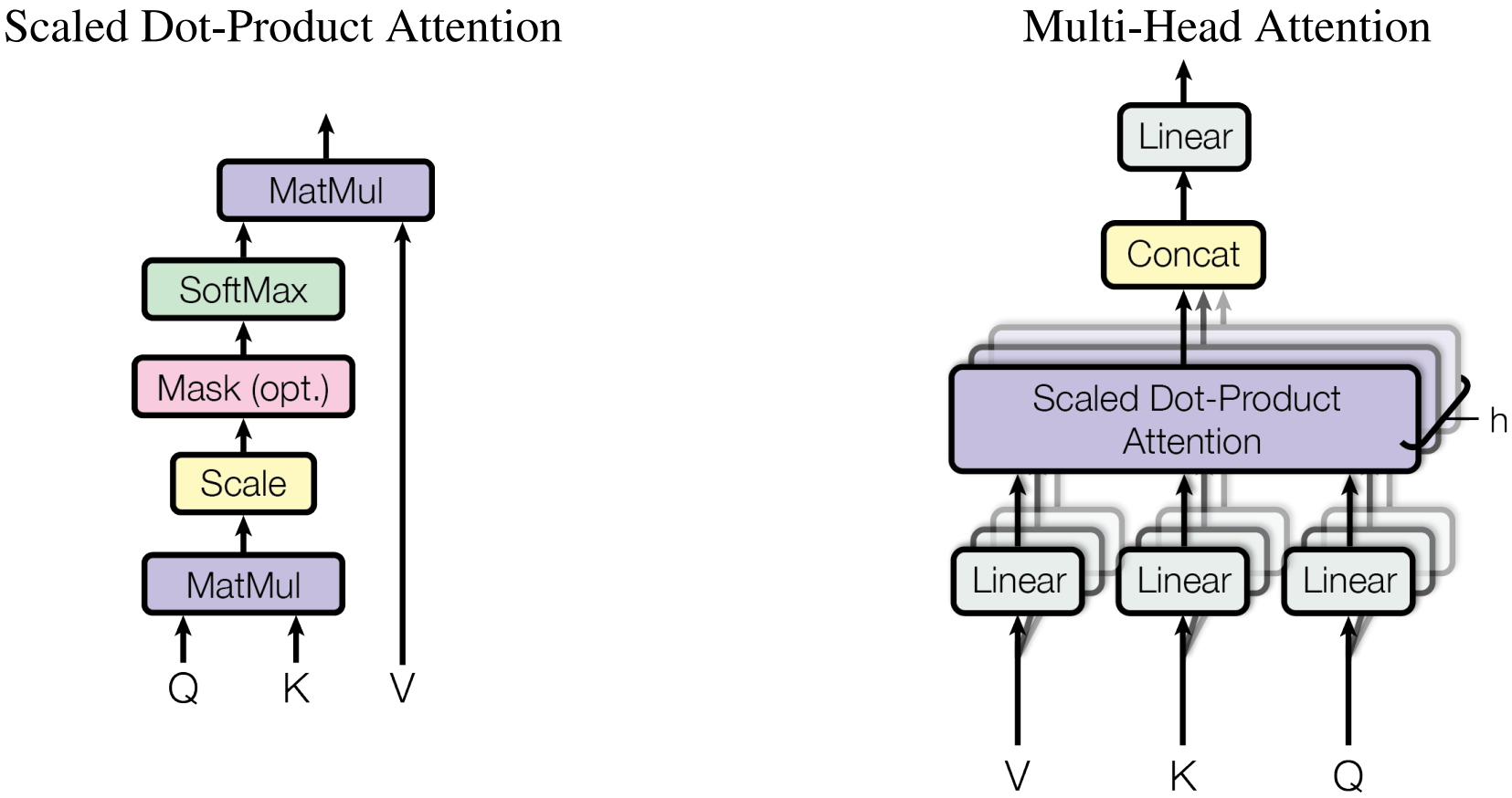


Figure: Multi-Head Attention **[Vaswani et al., 2017]**

Advanced Neural Networks: Attention

Multi-Head Attention: Formulas

$$Q \in \mathbb{R}^{n \times d},\ K \in \mathbb{R}^{m \times d},\ MultiHead \in \mathbb{R}^{n \times d_{model}},\ V \in \mathbb{R}^{m \times v}$$

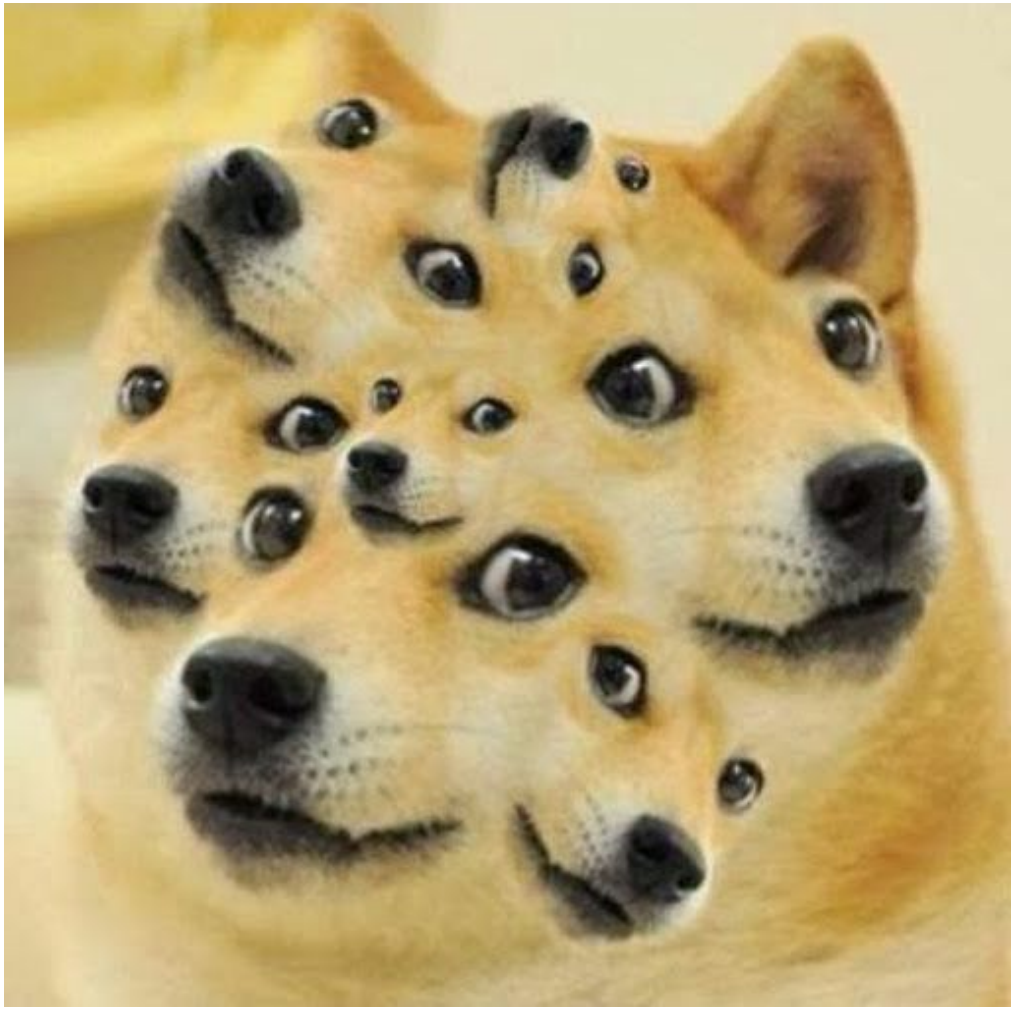
$$W_i^Q \in \mathbb{R}^{d_{model} \times d},\ W_i^K \in \mathbb{R}^{d_{model} \times d},\ W_i^V \in \mathbb{R}^{d_{model} \times v},\ W^O \in \mathbb{R}^{hv \times d_{model}}$$

$$head_i = Attention(QW_i^Q, KW_i^Q, VW_i^V)$$

$$MultiHead(Q, K, V) = Concat(head_1, \ldots, head_h) \cdot W^O$$

Advanced Neural Networks: Attention

Multi-Head Attention: Some humor



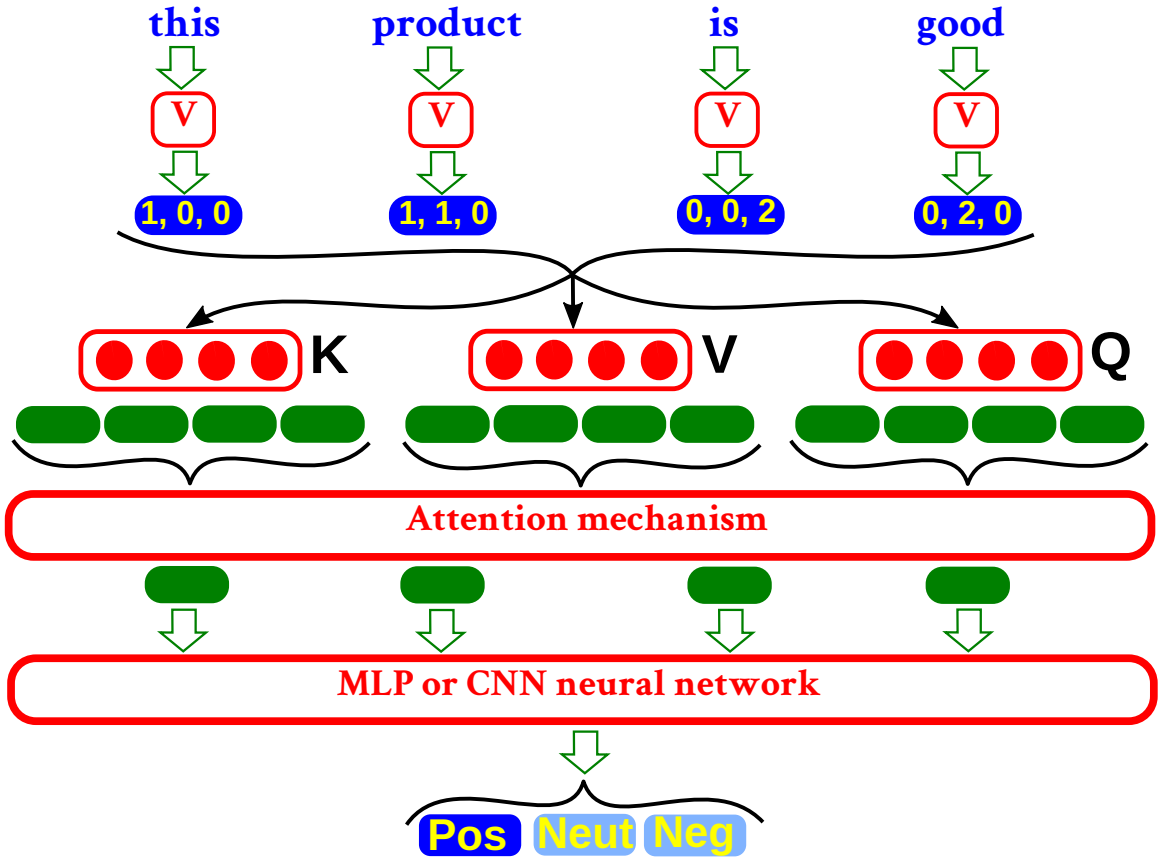
Advanced Neural Networks: Attention

Self-attention

- **GOAL**: Encode an element of a sequence with respect to the entire sequence.
- **Example**: Encode a word with respect to the sentence to capture its semantics.
- **Method**:
  - Use MLPs to learn the query, key, and value for each element.
  - Set the maximum number of elements in a sequence.
  - Truncate sequences that exceed this number.
  - Pad those that do not reach this number with a predefined code.
  - Optionally use multi-head attention to learn multiple representations.
  - Add positional embeddings to retain positional information in the sequence.

Advanced Neural Networks: Attention

Self-attention: Example



V Words' vectorization function (embedding)

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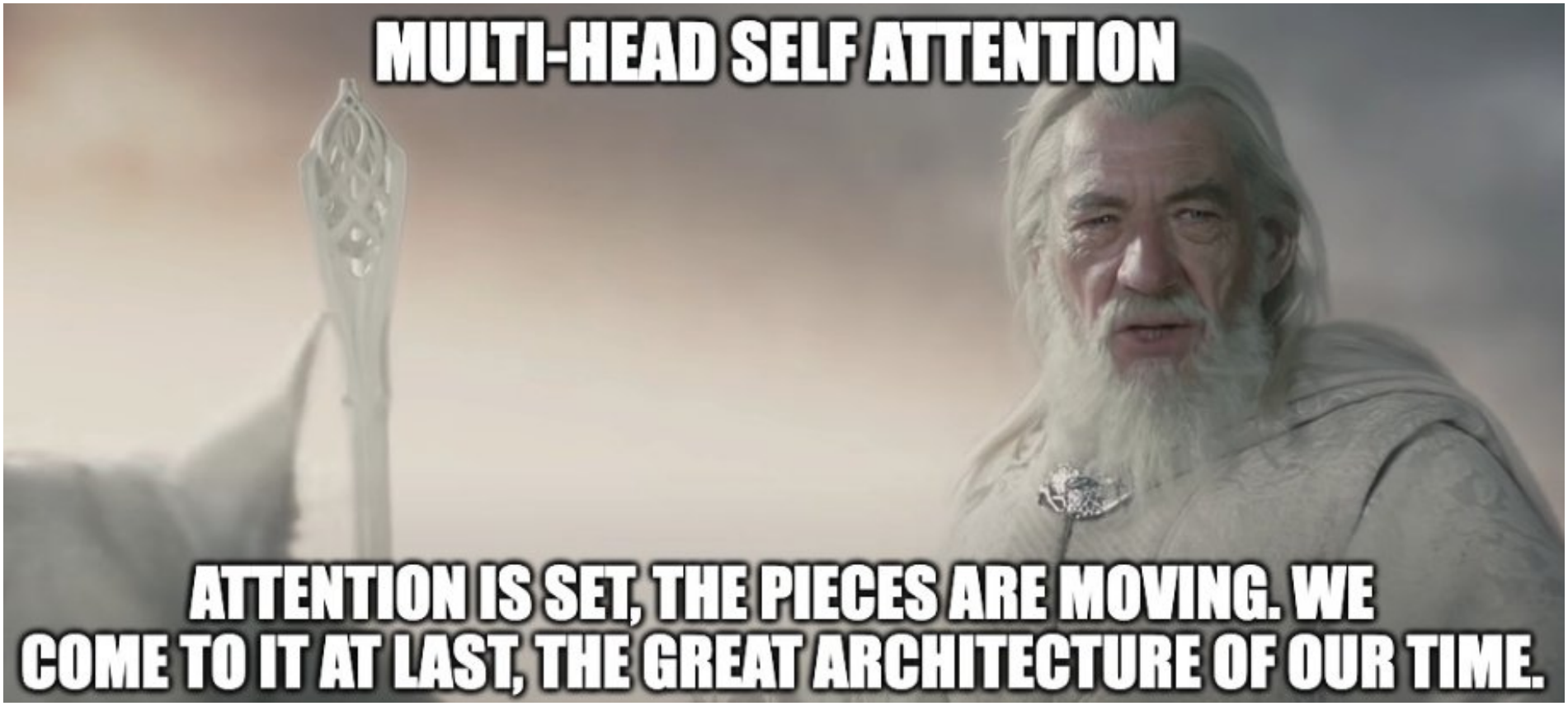
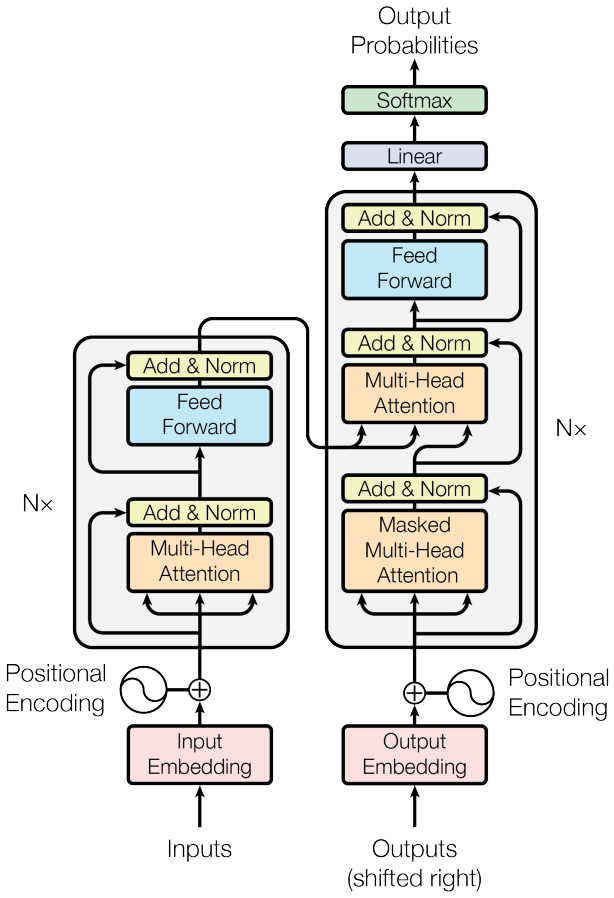
Self-attention: Some humor



Advanced Neural Networks: Attention

Transformer



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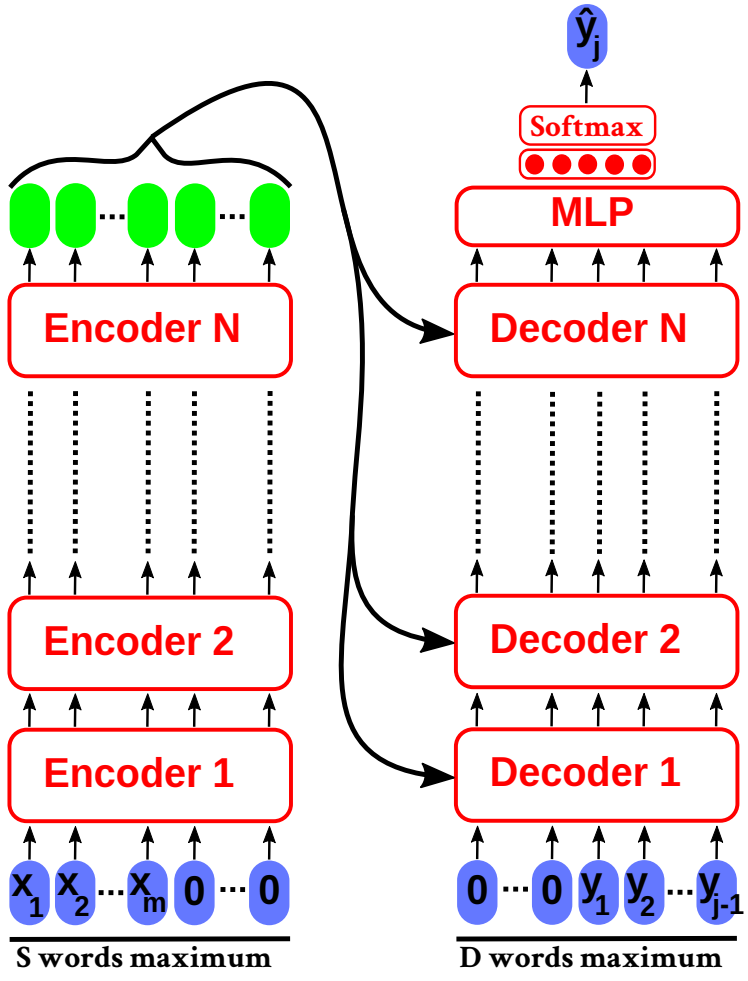


Figure: Transformers' architecture
[Vaswani et al., 2017]

Advanced Neural Networks: Attention

Transformer: Encoder

- Encodes each input element based on its context (the entire input).
- Uses multi-head self-attention
- Completely bi-directional
  - In BiRNN architecture, the encoder represents long-term relation indirectly (using a context).
  - In Encoders it is directly represented, but the notion of element's position is lost.
- We can introduce position's embedding into the word's initial representation (before being transformed into keys, values and queries).

Advanced Neural Networks: Attention

Transformer: Decoder

- ***Autoregressive***: The output is a **direct** function of the past elements

$$\hat{y}_t = \sum_{i=1}^{\rho} \varphi_i y_{t-i} + \epsilon_t$$

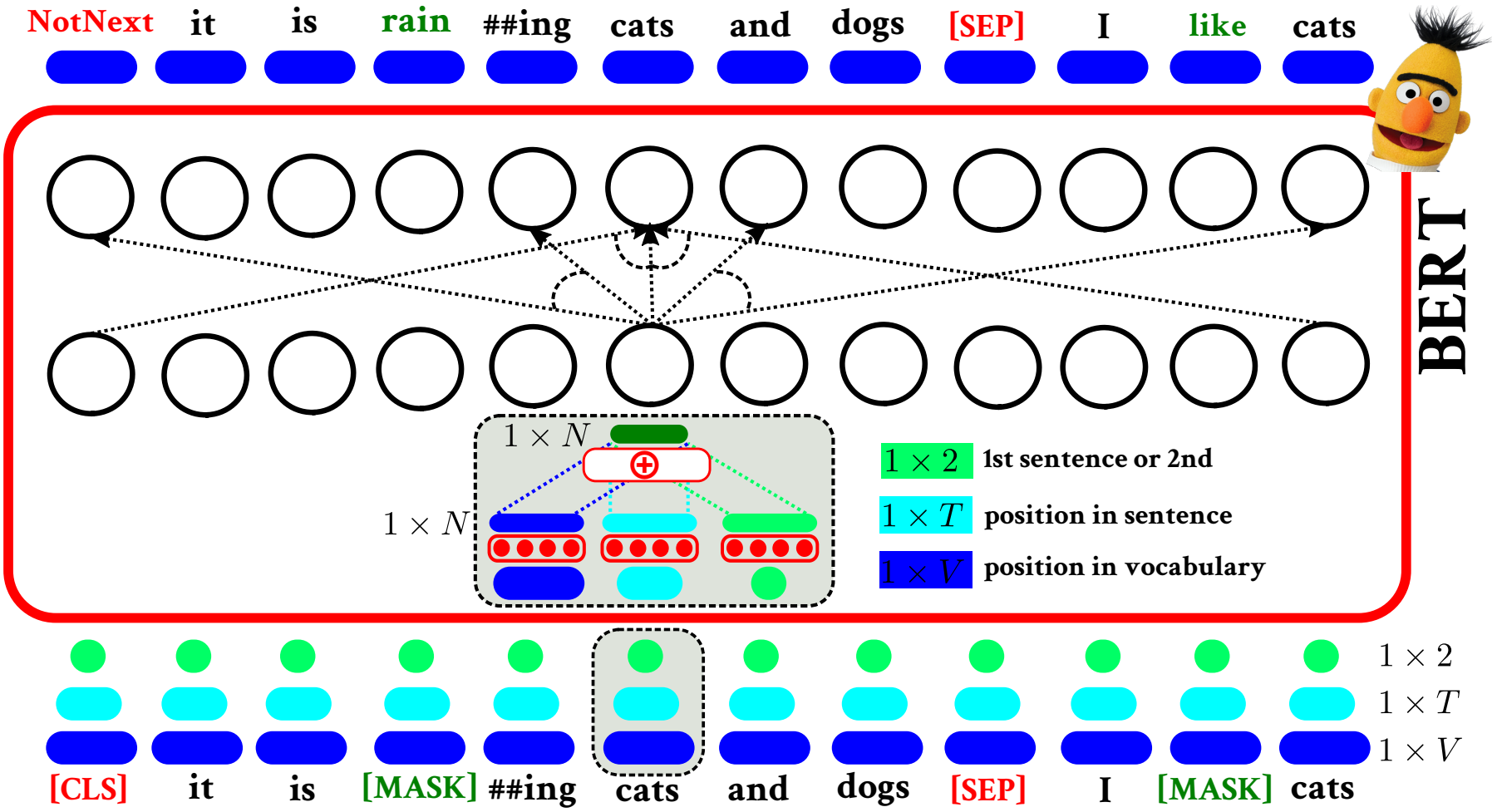
- Not as RNNs where the dependence is indirect

$$\hat{y}_t = \arg\max_y p(y|X;\ y_1, \cdots, y_{i-1};\ W;\ b)$$

- Each time an element is generated, it will be added into the input to generate the next element.
- To stop generating, a maximum size is used. Also, a special token is used to mark the end of generation.

Advanced Neural Networks: Attention

Transformer: Pretrained models (BERT: Enc) [Devlin et al., 2019]



Advanced Neural Networks: Attention

Transformer: Pretrained models (ViT: Enc) [Dosovitskiy et al., 2021]

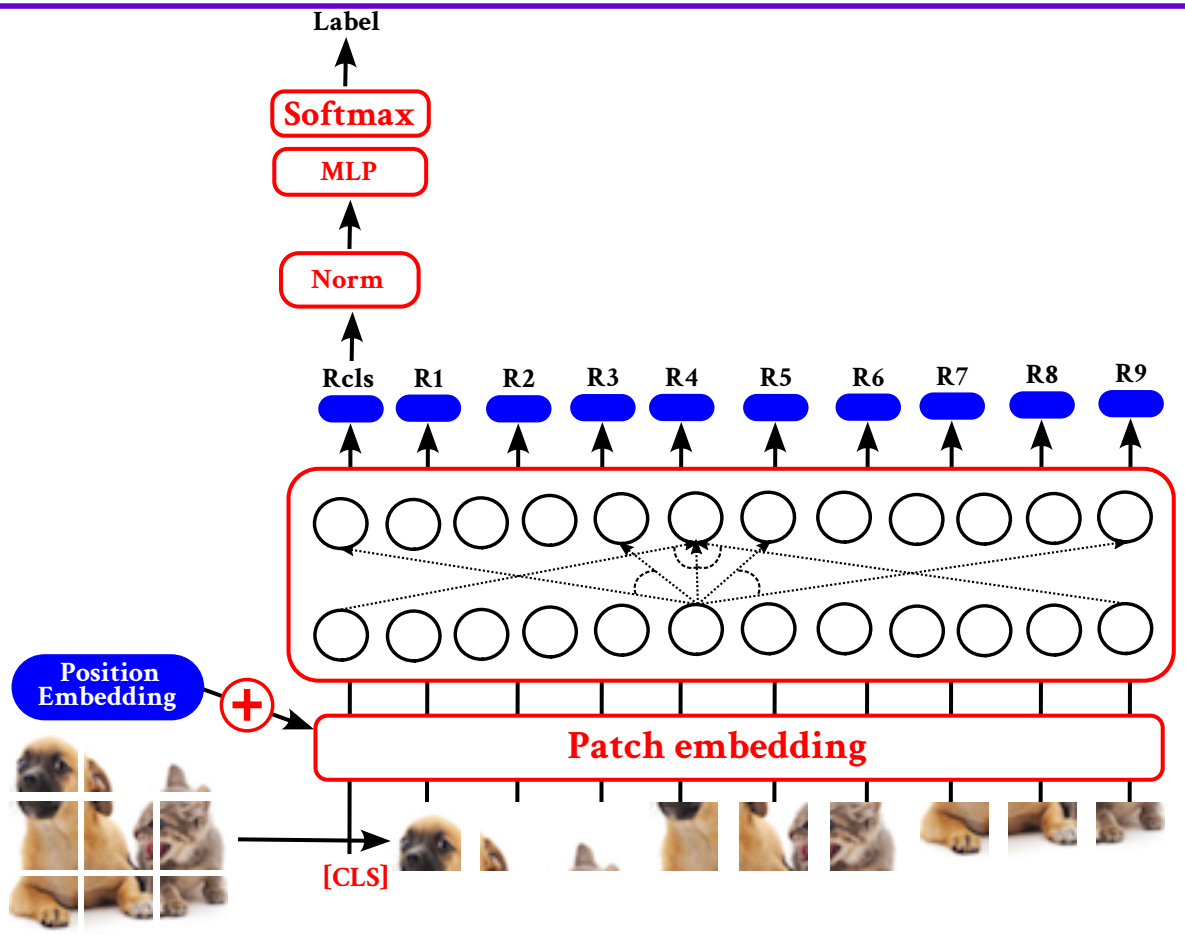


Figure: Example of images encoder [modified from [Zhang et al., 2021]]

Advanced Neural Networks: Attention

Transformer: Pretrained models (GPT: Dec) [Radford et al., 2018]

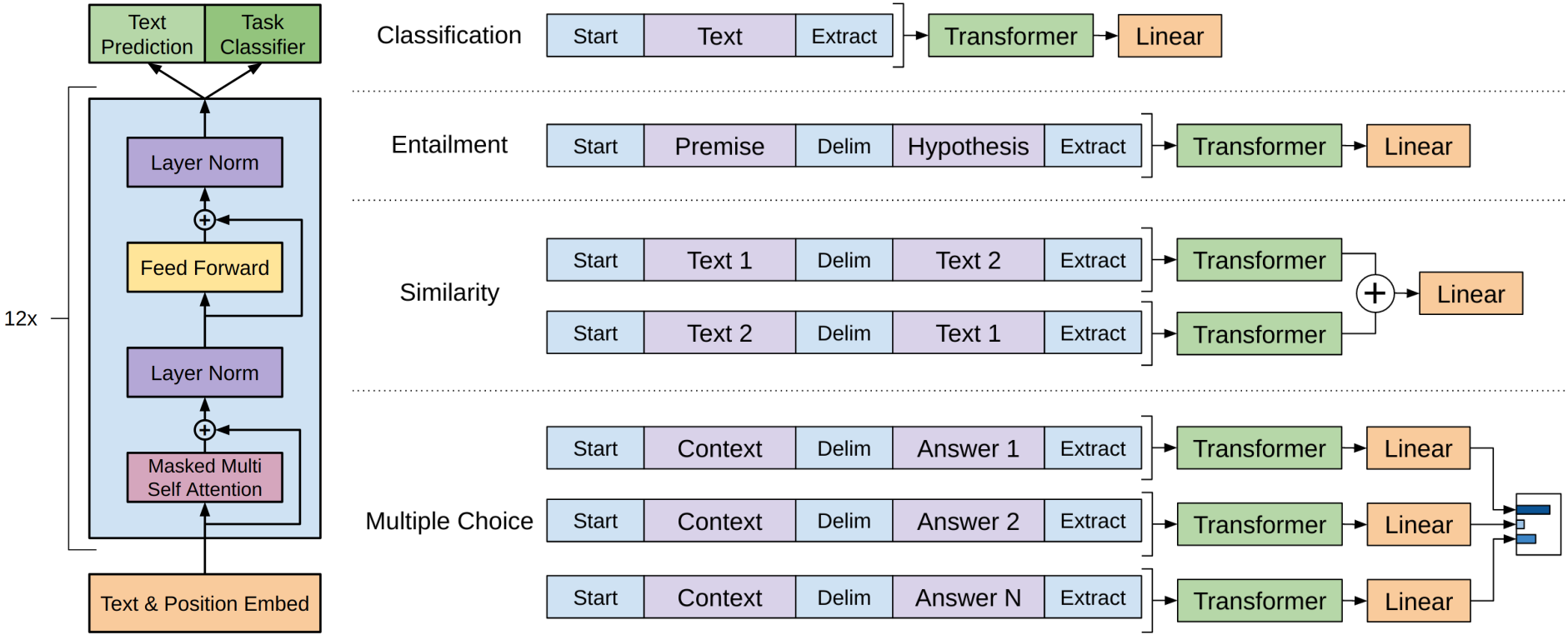


Figure: GPT's architecture and different tasks [Radford et al., 2018]

Advanced Neural Networks: Attention

Transformer: Pretrained models (T5: Enc-Dec) [Raffel et al., 2020]

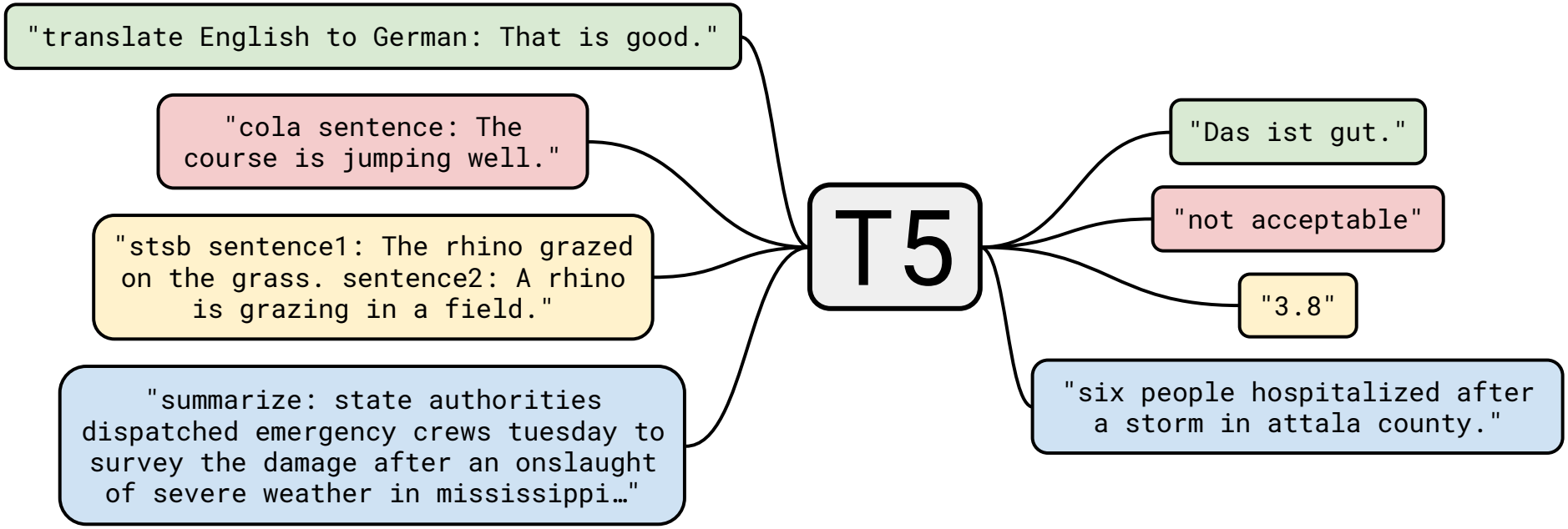


Figure: T5 (Text-to-Text Transfer Transformer) training [Raffel et al., 2020]

Advanced Neural Networks: Attention

Transformer: Pretrained models (BART: Enc-Dec) [Lewis et al., 2020]

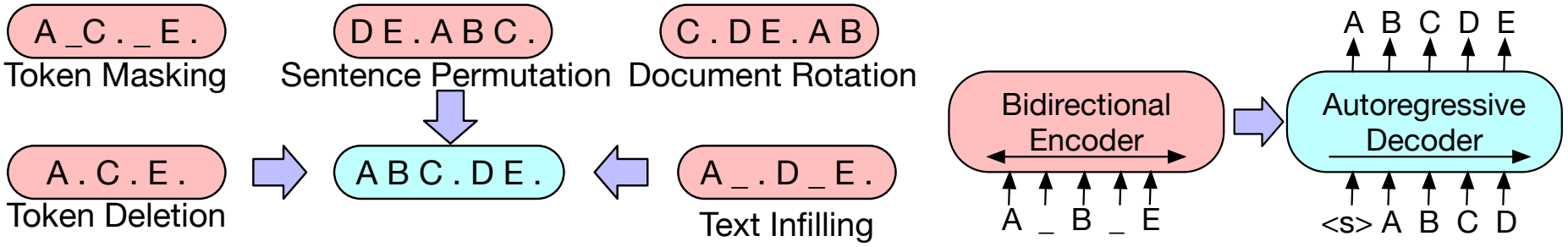


Figure: BART training [Lewis et al., 2020]

Advanced Neural Networks: Attention

Transformer: Some humor

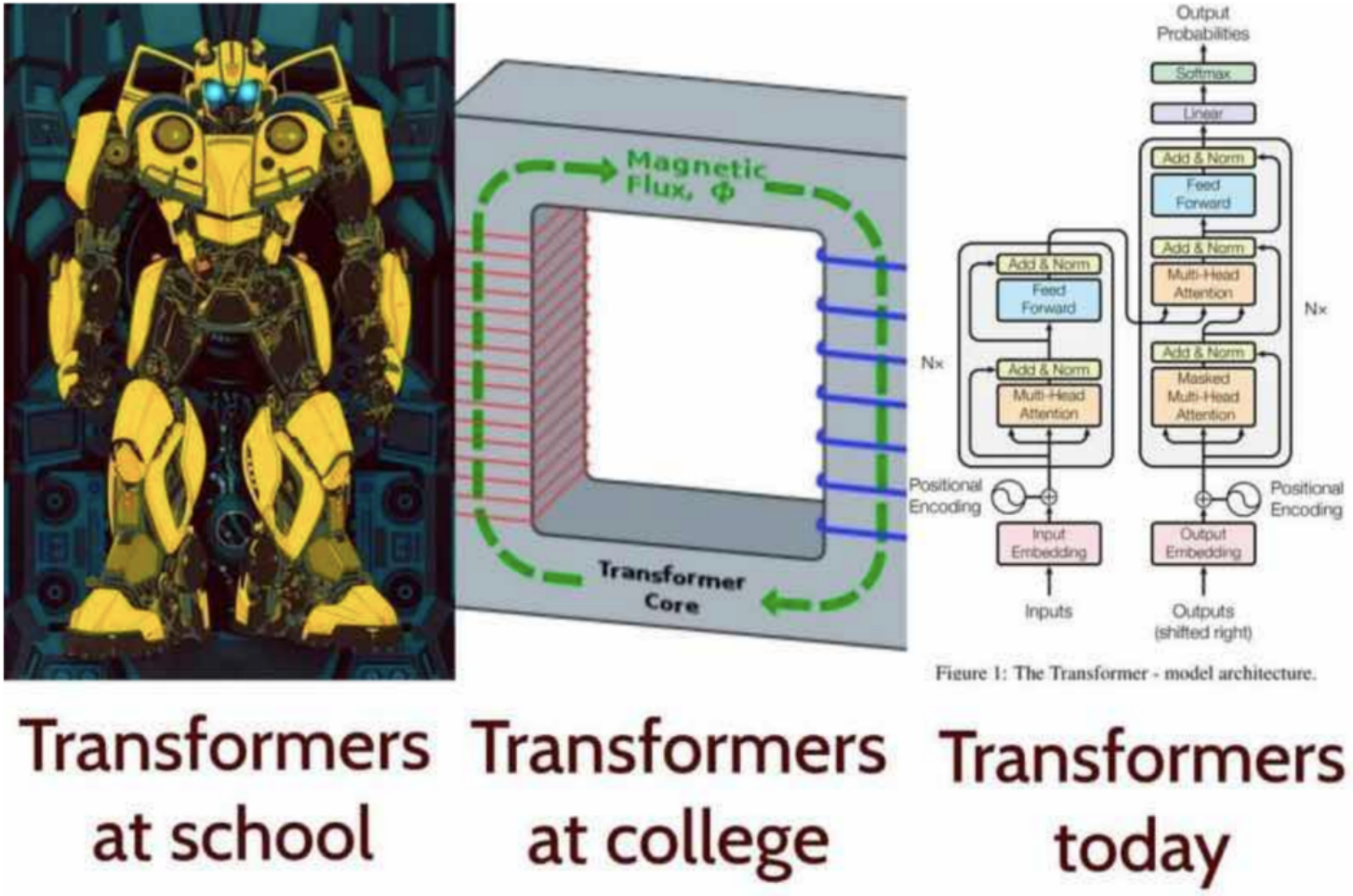


Figure 1: The Transformer - model architecture.

Section 5

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THIS IS A NEURAL NETWORK.

IT MAKES MISTAKES.
IT LEARNS FROM THEM.

BE LIKE A NEURAL NETWORK.