Deep Learning with R

Neural network fundamentals

Mikhail Dozmorov

Virginia Commonwealth University

2020-06-08

Deep Learning Prerequisites

For each machine- and deep learning algorithms, we need:

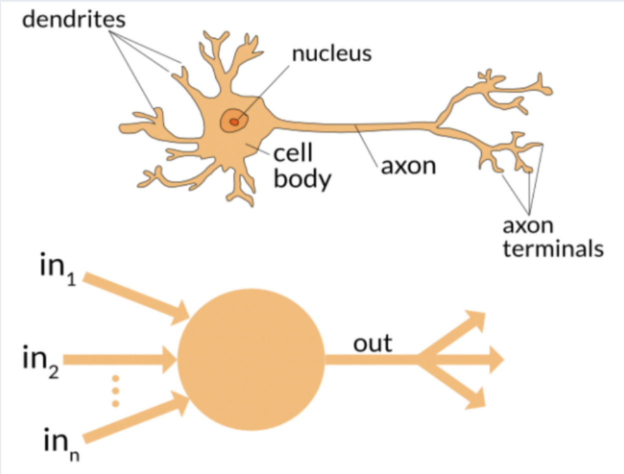
- **Input data** - samples and their properties. E.g., images represented by color pixels. Proper data representation is crucial
- **Examples of the expected output** - expected sample annotations
- **Performance evaluation metrics** - how well the algorithm's output matches the expected output. Used as a feedback signal to adjust the algorithm - the process of learning

How deep learning learns

- Creates layer-by-layer increasingly complex representations of the input data maximizing learning accuracy
- Intermediate representations learned jointly, with the properties of each layer being updated depending on the following and the previous layers

The beginning of Deep Learning

- A generic Deep Learning architecture is made up of a combination of several layers of "neurons"
- The concept of a "neuron" was proposed in the 1950s with the well-known Rosenblatt "perceptron", inspired by brain function
- The **multilayer perceptron (MLP)** is a fully-connected feedforward neural network containing at least one hidden layer

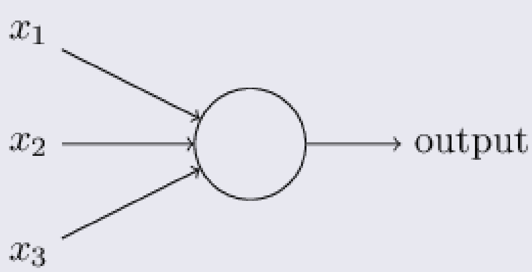


Deep Learning winter and revival

- Widespread belief that gradient descent would be unable to escape poor local minima during optimization, preventing neural networks from converging to a global acceptable solution
- During 1980s, 1990s, deep neural networks were largely abandoned
- In 2006, deep belief networks revived interest to deep learning
- In 2012, Krizhevsky et al. presented a convolutional neural network that significantly improved image recognition accuracy
- GPU technologies enabled further development

Hinton GE, Osindero S, Teh Y-W. A fast learning algorithm for deep belief nets. Neural Comput. 2006

The Perceptron: Linear input-output relationships

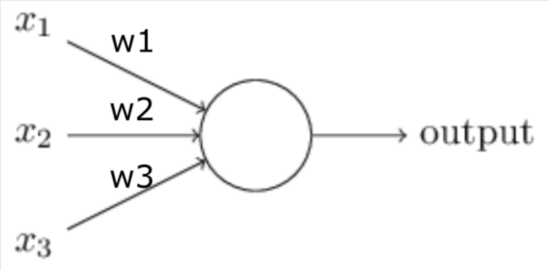


- Input: Take $x_1 = 0$, $x_2 = 1$, $x_3 = 1$ and setting a $threshold = 0$
- If $x_1 + x_2 + x_3 > 0$, the output is 1 otherwise 0
- Output: calculated as 1

https://www.analyticsvidhya.com/blog/2017/05/neural-network-from-scratch-in-python-and-r/

http://neuralnetworksanddeeplearning.com/chap1.html

The Perceptron: Adding weights to inputs

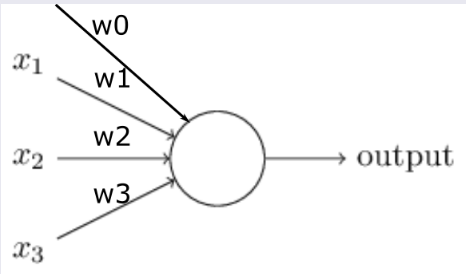


$\hat{y} = g(\sum_{i=1}^{m} x_i w_i)$

- $\hat{y}$ - the output
- $\sum$ - the linear combination of inputs
- g - a non-linear activation function

- Weights give importance to an input. For example, you assign $w_1 = 2$, $w_2 = 3$ and $w_3 = 4$ to x_1, x_2 and x_3 respectively. These weights assign more importance to x_3.
- To compute the output, we will multiply input with respective weights and compare with threshold value as $w_1 * x_1 + w_2 * x_2 + w_3 * x_3 > threshold$

The Perceptron: Adding bias



$\hat{y} = g(w_0 + \sum_{i=1}^{m} x_i w_i)$

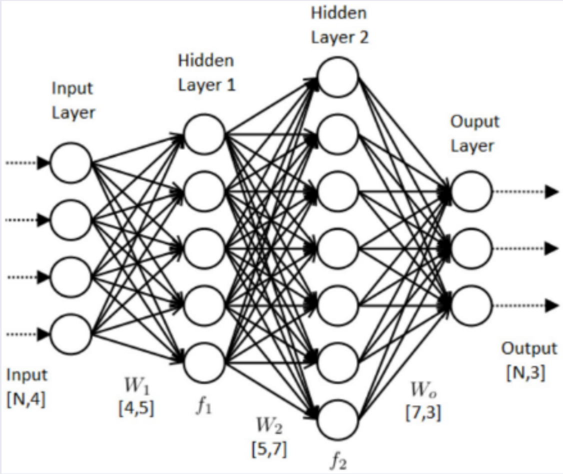
- w_0 - bias term

$\hat{y} = g(w_0 + X^T W)$

- Bias adds flexibility to the perceptron by globally shifting the calculations and allowing the weights to be more precise
- Think about a linear function $y = ax + b$, where b is the bias. Without bias, the line will always go through the origin (0,0) and we get poorer fit
- Input consists of multiple values x_i and multiple weights w_i, but only one bias is added. For $i = 3$, the linear representation of input will look like $w_1 * x_1 + w_2 * x_2 + w_3 * x_3 + 1 * b$

https://www.analyticsvidhya.com/blog/2017/05/neural-network-from-scratch-in-python-and-r/

Multi-layer neural network



- **Input** - a layer with n neurons each taking input measures
- **Processing information** - each neuron maps input to output via nonlinear transformations that include input data x_i, weights w_i, and biases b

Layers

- Deep learning models are formed by multiple layers
- The multi-layer perceptron (MLP) with more than 2 hidden layers is already a Deep Model
- Most frequently used layers
  - Convolution Layer
  - Max/Average Pooling Layer
  - Dropout Layer
  - Batch Normalization Layer
  - Fully Connected (Affine) Layer
  - Relu, Tanh, Sigmoid Layer (Non-Linearity Layers)
  - Softmax, Cross-Entropy, SVM, Euclidean (Loss Layers)

Fitting the parameters using the training set

- Parameters of the neural network (weights and biases) are first *randomly initialized*
  - For a given layer, initialize weights using Gaussian random variables with $\mu = 0$ and $\sigma = 1$
  - Better to use standard deviation $1/\sqrt{n_{neurons}}$
  - Uniform distribution, and its modifications, also used
- Small random subsets, so-called batches, of input–target pairs of the training data set are iteratively used to make small updates on model parameters to minimize the loss function between the predicted values and the observed targets
- This minimization is performed by using the gradient of the loss function computed using the backpropagation algorithm

Overflow and underflow

- Need to represent infinitely many real numbers with a finite number of fig patterns
- The approximation error is always present and can accumulate across many operations
- **Underflow** occurs when numbers near zero are rounded to zero
- **Overflow** occurs when numbers with large magnitude are approximated as ∞ or $-\infty$

Activation function

Activation function takes the sum of weighted inputs as an argument and returns the output of the neuron

$$a = f(\sum_{i=0}^{N} w_i x_i)$$

where index 0 correspond to the bias term ($x_0 = b$, $w_0 = 1$).

Activation functions

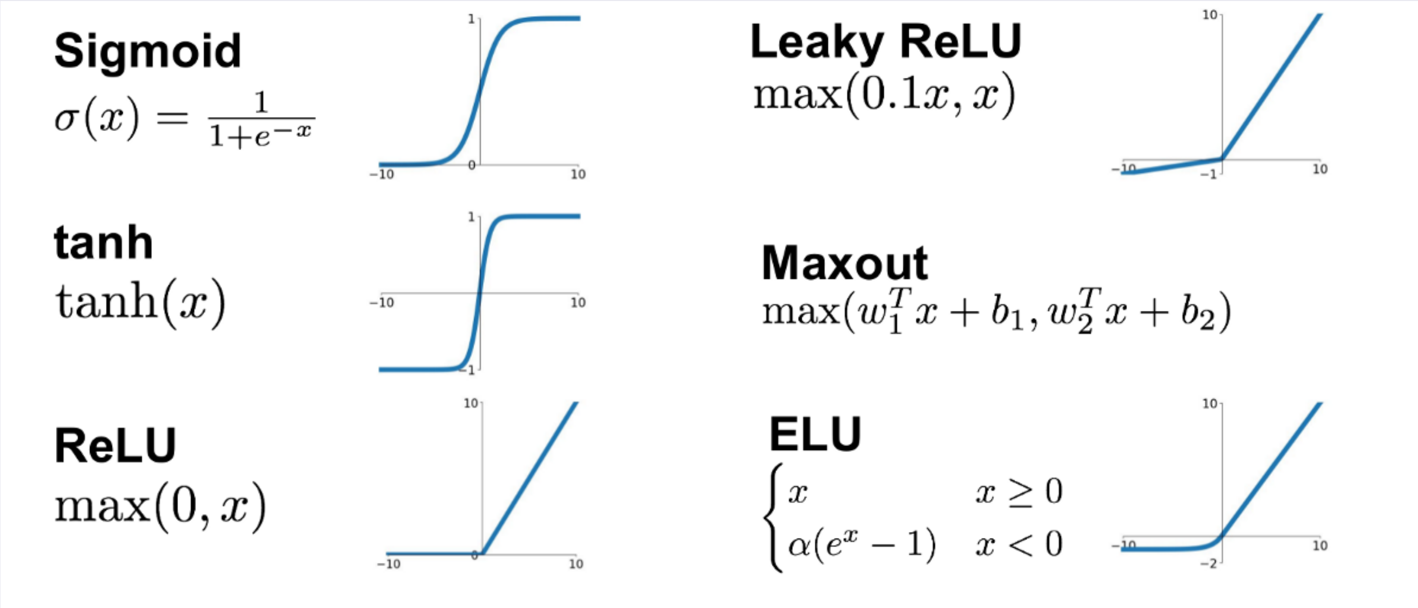
- Adds nonlinearity to the network calculations, allows for flexibility to capture complex nonlinear relationships
- **Softmax** - applied over a vector $z = (z_1, \ldots, z_K) \in R^K$ of length K as $\sigma(z)_i = \frac{e^{z_i}}{\sum_{j=1}^{K} e^{z_j}}$
- **Sigmoid** - $f(x) = \frac{1}{1+e^{-x}}$
- **Tahn** - Hyperbolic tangent $tanh(x) = 2 * sigmoid(2x) - 1$
- **ReLU** - Rectified Linear Unit $f(x) = max(x, 0)$.

Other functions: binary step function, linear (i.e., identity) activation function, exponential and scaled exponential linear unit, softplus, softsign

https://keras.io/activations/

https://www.analyticsvidhya.com/blog/2020/01/fundamentals-deep-learning-activation-functions-when-to-use-them/

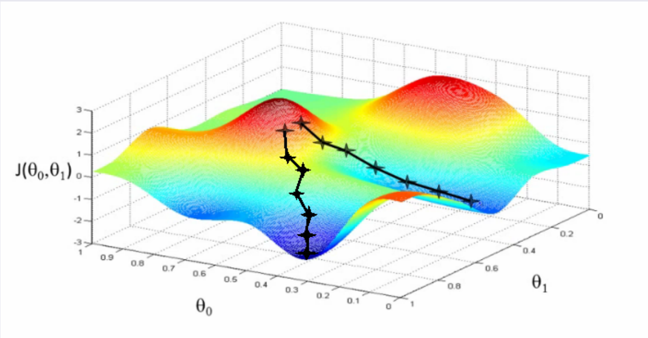
Activation functions overview



https://towardsdatascience.com/complete-guide-of-activation-functions-34076e95d044

Learning rules

- **Optimization** - update model parameters on the training data and check its performance on a new validation data to find the most optimal parameters for the best model performance



https://www.youtube.com/watch?v=5u4G23_OohI

https://www.analyticsvidhya.com/blog/2017/03/introduction-to-gradient-descent-algorithm-along-its-variants/

Loss function

- **Loss function** - (aka objective, or cost function) metric to assess the predictive accuracy, the difference between true and predicted values. Needs to be minimized (or, maximized, metric-dependent)
  - **Regression loss functions** - mean squared error (MSE) $MSE = \frac{1}{n}\sum_{i=1}^{n}(Y_i - \hat{Y}_i)^2$
  - **Binary classification loss functions** - Binary Cross-Entropy $-(ylog(p) + (1-y)log(1-p))$
  - **Multi-class classification loss functions** - Multi-class Cross Entropy Loss $-\sum_{c=1}^{M} y_{o,c}log(p_{o,c})$ (M - number of classes, y - binary indicator if class label c is the correct classification for observation o, p - predicted probability observation o is of class c), Kullback-Leibler Divergence Loss $\sum \hat{y} * log(\frac{\hat{y}}{y})$

https://ml-cheatsheet.readthedocs.io/en/latest/loss_functions.html

Loss optimization

We want to find the network weights that achieve the lowest loss

$$W^* = \arg\min_{W} \frac{1}{n} \sum_{i=1}^{n} L(f(x^{(i)}; W), y^{(i)})$$

where $W = \{W^{(0)}, W^{(1)}, \dots\}$

Gradient descent

- An optimization technique - finds a combination of weights for best model performance
- **Full batch gradient descent** uses all the training data to update the weights
- **Stochastic gradient descent** uses parts of the training data
- Gradient descent requires calculation of gradient by differentiation of cost function. We can either use first-order differentiation or second-order differentiation

https://www.analyticsvidhya.com/blog/2017/03/introduction-to-gradient-descent-algorithm-along-its-variants/

Richards, Blake A., Timothy P. Lillicrap, Philippe Beaudoin, Yoshua Bengio, Rafal Bogacz, Amelia Christensen, Claudia Clopath, et al. "A Deep Learning Framework for Neuroscience." Nature Neuroscience 2019 - Box 1, Learning and the credit assignment problem

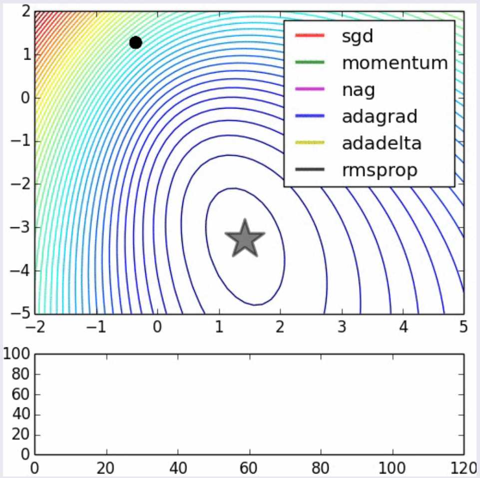
Gradient descent algorithm

- Initialize weights randomly $\sim N(0, \sigma^2)$
- Loop until convergence
  - Compute gradient, $\frac{\partial J(W)}{\partial W}$
  - Update weights, $W \leftarrow W - \eta \frac{\partial J(W)}{\partial W}$
- Return weights

where η is a learning rate. Right selection is critical - too small may lead to local minima, too large may miss minima entirely. Adaptive implementations exist

Gradient descent algorithms

- Stochastic Gradient Descent (**SGD**)
- Stochastic Gradient Descent with momentum (Very popular)
- Nesterov's accelerated gradient (NAG)
- Adaptive gradient (**AdaGrad**)
- **Adam** (Very good because you need to take less care about learning rate)
- **RMSprop**



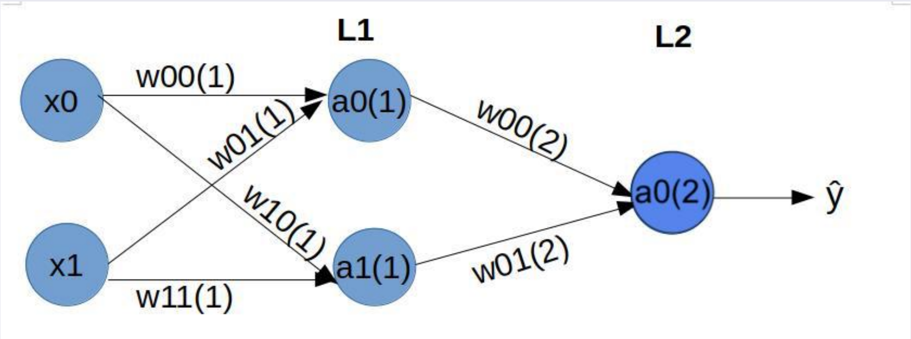
https://leonardoaraujosantos.gitbooks.io/artificial-inteligence/model_optimization.html

Forward and backward propagation

- Forward propagation computes the output by passing the input data through the network
- The estimated output is compared with the expected output - the error (loss function) is calculated
- Backpropagation (the chain rule) propagates the loss back through the network and updates the weights to minimize the loss. Uses chain rule to recursively calculate gradients backward from the output
- Each round of forward- and backpropagation is known as one training iteration or epoch

Rumelhart, David E, Geoffrey E Hinton, and Ronald J Williams. "Learning Representations by Back-Propagating Errors," 1986

Forward propagation

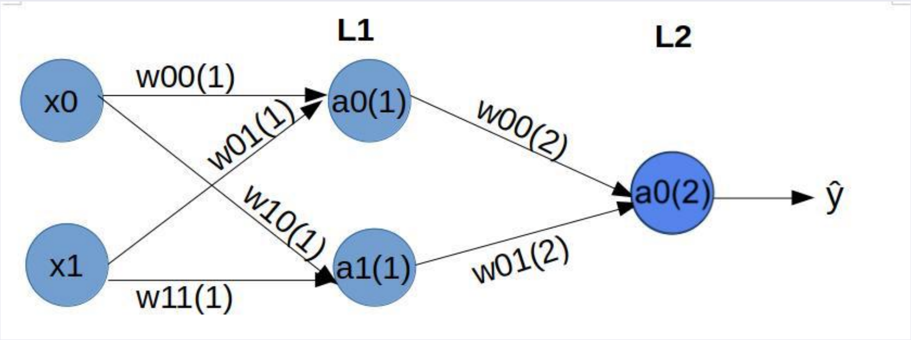


Assuming sigmoid activation function $\sigma(f)$, at Layer L1, we have:

$$a_0^1 = \sigma([w_{00}^1 \cdot x_0 + b_{00}^1] + [w_{01}^1 \cdot x_1 + b_{01}^1])$$

$$a_1^1 = \sigma([w_{10}^1 \cdot x_0 + b_{10}^1] + [w_{11}^1 \cdot x_1 + b_{11}^1])$$

Forward propagation



At Layer L2, we have:

$$\hat{y} = \sigma([w_{00}^2 \cdot a_0^1 + b_{00}^2] + [w_{01}^2 \cdot a_1^1 + b_{01}^2])$$

https://www.analyticsvidhya.com/blog/2020/04/comprehensive-popular-deep-learning-interview-questions-answers/

Backpropagation

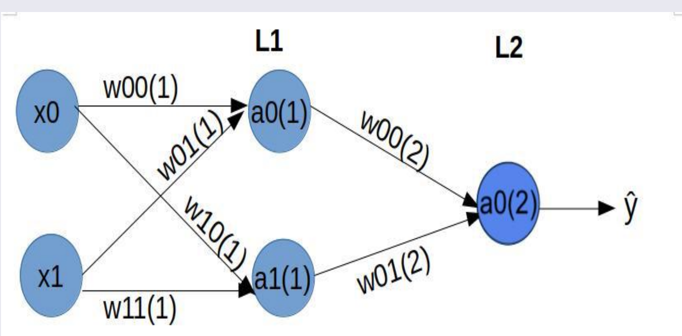
Back-propagation - A common method to train neural networks by updating its parameters (i.e., weights) by using the derivative of the network's performance with respect to the parameters. A technique to calculate gradient through the chain of functions

$$\frac{\partial J(W)}{\partial w_1} = \frac{\partial J(W)}{\partial \hat{y}} * \frac{\partial \hat{y}}{\partial z_1} * \frac{\partial z_1}{\partial w_1}$$

Review https://ml-cheatsheet.readthedocs.io/en/latest/backpropagation.html

Rumelhart, David E, Geoffrey E Hinton, and Ronald J Williams. "Learning Representations by Back-Propagating Errors", 1986, 4.

Backpropagation



At Layer L2,

$$\frac{\delta C}{\delta w_{00}^{(2)}} = \frac{\delta C}{\delta a_0^{(2)}} \cdot \frac{\delta a_0^{(2)}}{\delta z_0^{(2)}} \cdot \frac{\delta z_0^{(2)}}{\delta w_{00}^{(2)}}$$

$$\frac{\delta C}{\delta w_{01}^{(2)}} = \frac{\delta C}{\delta a_0^{(2)}} \cdot \frac{\delta a_0^{(2)}}{\delta z_0^{(2)}} \cdot \frac{\delta z_0^{(2)}}{\delta w_{01}^{(2)}}$$

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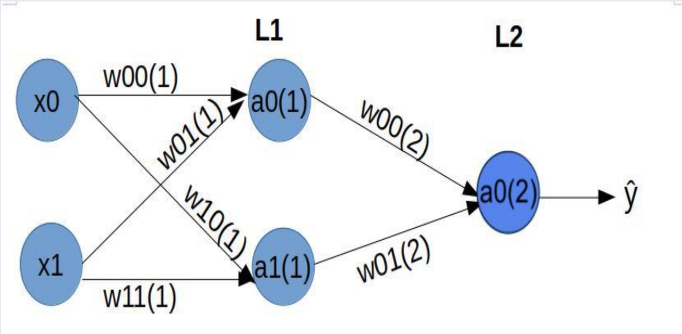
Backpropagation



At Layer L1,

1.

$$\frac{\delta C}{\delta w_{00}^{(1)}}=\frac{\delta C}{\delta a_0^{(1)}}\cdot\frac{\delta a_0^{(1)}}{\delta z_0^{(1)}}\cdot\frac{\delta z_0^{(1)}}{\delta w_{00}^{(1)}}=[\frac{\delta C}{\delta a_0^{(2)}}\cdot\frac{\delta a_0^{(2)}}{\delta z_0^{(2)}}\cdot\frac{\delta z_0^{(2)}}{\delta a_0^{(1)}}]\cdot\frac{\delta a_0^{(1)}}{\delta z_0^{(1)}}\cdot\frac{\delta z_0^{(1)}}{\delta w_{00}^{(1)}}$$

2.

$$\frac{\delta C}{\delta w_{01}^{(1)}}=\frac{\delta C}{\delta a_0^{(1)}}\cdot\frac{\delta a_0^{(1)}}{\delta z_0^{(1)}}\cdot\frac{\delta z_0^{(1)}}{\delta w_{01}^{(1)}}=[\frac{\delta C}{\delta a_0^{(2)}}\cdot\frac{\delta a_0^{(2)}}{\delta z_0^{(2)}}\cdot\frac{\delta z_0^{(2)}}{\delta a_0^{(1)}}]\cdot\frac{\delta a_0^{(1)}}{\delta z_0^{(1)}}\cdot\frac{\delta z_0^{(1)}}{\delta w_{01}^{(1)}}$$

3.

$$\frac{\delta C}{\delta w_{10}^{(1)}}=\frac{\delta C}{\delta a_1^{(1)}}\cdot\frac{\delta a_1^{(1)}}{\delta z_1^{(1)}}\cdot\frac{\delta z_1^{(1)}}{\delta w_{10}^{(1)}}=[\frac{\delta C}{\delta a_0^{(2)}}\cdot\frac{\delta a_0^{(2)}}{\delta z_0^{(2)}}\cdot\frac{\delta z_0^{(2)}}{\delta a_1^{(1)}}]\cdot\frac{\delta a_0^{(1)}}{\delta z_0^{(1)}}\cdot\frac{\delta z_0^{(1)}}{\delta w_{00}^{(1)}}$$

4.

$$\frac{\delta C}{\delta w_{11}^{(1)}}=\frac{\delta C}{\delta a_1^{(1)}}\cdot\frac{\delta a_1^{(1)}}{\delta z_1^{(1)}}\cdot\frac{\delta z_1^{(1)}}{\delta w_{11}^{(1)}}=[\frac{\delta C}{\delta a_0^{(2)}}\cdot\frac{\delta a_0^{(2)}}{\delta z_0^{(2)}}\cdot\frac{\delta z_0^{(2)}}{\delta a_1^{(1)}}]\cdot\frac{\delta a_0^{(1)}}{\delta z_0^{(1)}}\cdot\frac{\delta z_0^{(1)}}{\delta w_{11}^{(1)}}$$

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Backpropagation Explained

A series of 10-15 min videos by deeplizard

- Part 1 - The Intuition
- Part 2 - The Mathematical Notation
- Part 3 - Mathematical Observations and the chain rule
- Part 4 - Calculating The Gradient, derivative of the loss function with respect to the weights
- Part 5 - What Puts The "Back" In Backprop?

Analytics Vidhya tutorial: Step-by-step forward and backpropagation, implemented in R and Python: https://www.analyticsvidhya.com/blog/2017/05/neural-network-from-scratch-in-python-and-r/

Vanishing gradient

- Typical deep NNs suffer from the problem of vanishing or exploding gradients
  - The gradient descent tries to minimize the error by taking small steps towards the minimum value. These steps are used to update the weights and biases in a neural network
  - On the course of backpropagation, the steps may become too small, resulting in negligible updates to weights and bias terms. Thus, a network will be trained with nearly unchanging weights. This is the **vanishing gradient** problem
  - Weights of early layers (latest to be updated) suffer the most

https://en.wikipedia.org/wiki/Vanishing_gradient_problem

Vanishing & Exploding Gradient Explained | A Problem Resulting From Backpropagation

https://www.analyticsvidhya.com/blog/2020/04/comprehensive-popular-deep-learning-interview-questions-answers/

Exploding gradient

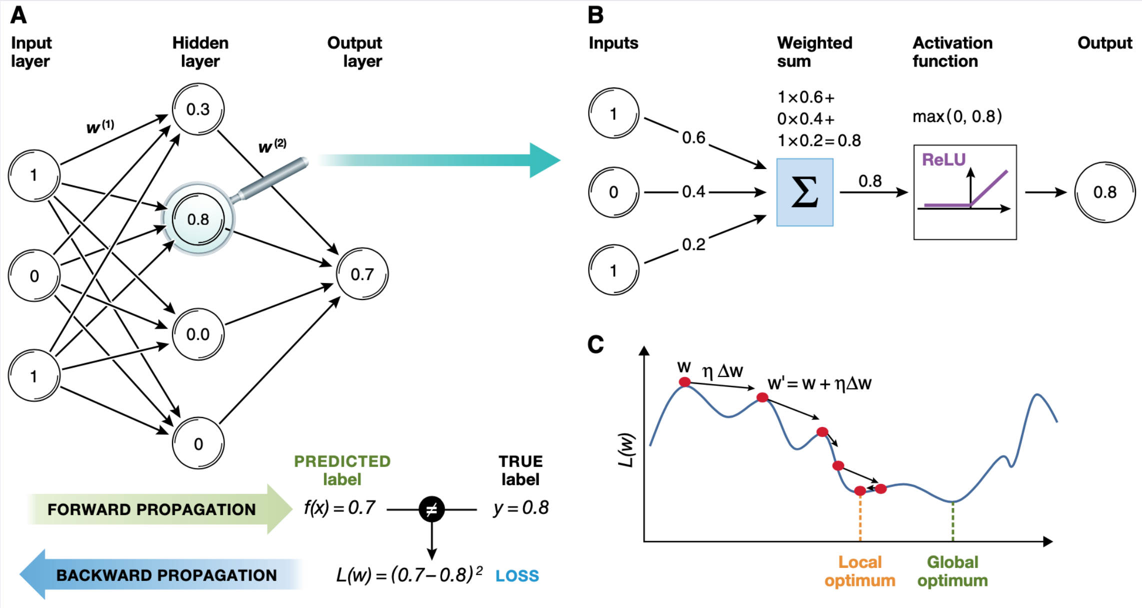
- Typical deep NNs suffer from the problem of vanishing or exploding gradients
  - The gradient descent tries to minimize the error by taking small steps towards the minimum value. These steps are used to update the weights and biases in a neural network
  - The steps may become too large, resulting in large updates to weights and bias terms and potential numerical overflow. This is the **exploding gradient** problem
  - Various solutions exist, typically by propagating a feedback signal from previous layers (residual connections)

https://en.wikipedia.org/wiki/Vanishing_gradient_problem

Vanishing & Exploding Gradient Explained | A Problem Resulting From Backpropagation

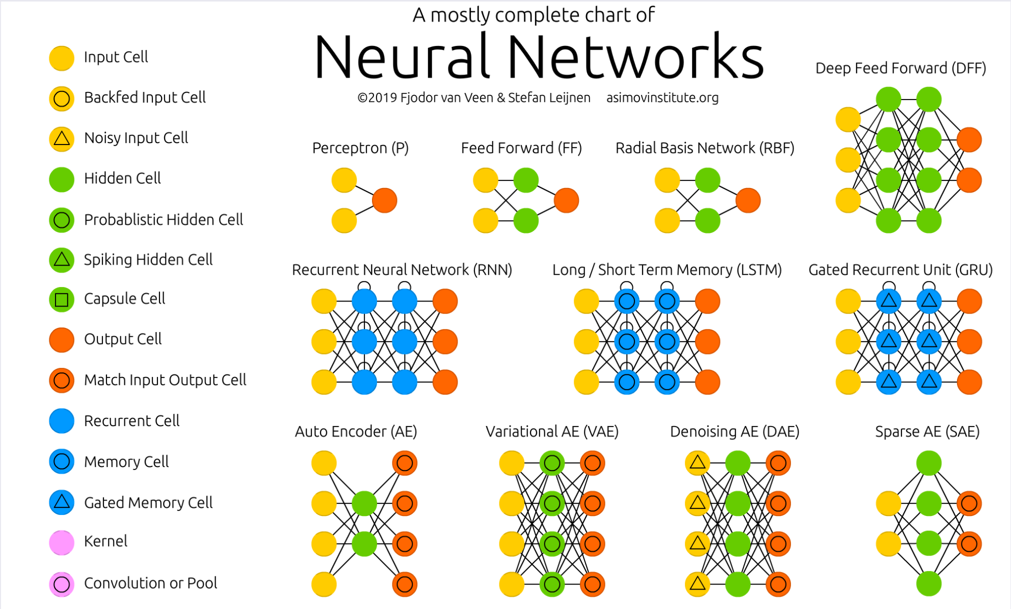
https://www.analyticsvidhya.com/blog/2020/04/comprehensive-popular-deep-learning-interview-questions-answers/

Neural Network summary



Angermueller et al., “Deep Learning for Computational Biology.”

The Neural Network Zoo



Review the complete infographics at https://www.asimovinstitute.org/neural-network-zoo/