Deep Learning

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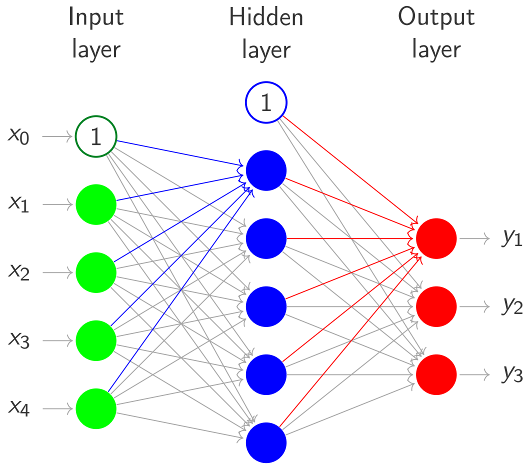
Training Neural Networks: Forward and Backward Propagation

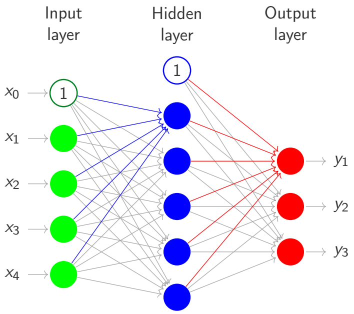
Neural Networks



Output of a neural network can be visualised graphically as *forward propagation of information*.

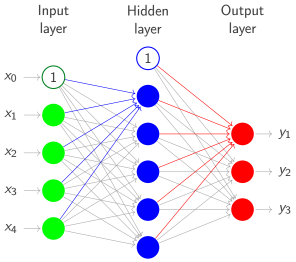
Neural Networks
Notation

- Input layer neurons will be indexed by i.
- Hidden layer neurons will be indexed by j.
- Next hidden layer or output layer neurons will be indexed by k.
- Weights of j-th hidden neuron will be denoted by the vector $\mathbf{w}_j^{(1)} \in \mathbb{R}^D$.
- Weight between i-th input neuron and j-th hidden neuron is $w_{ji}^{(1)}$.
- Weights of k-th output neuron will be denoted by the vector $\mathbf{w}_k^{(2)} \in \mathbb{R}^M$.
- Weight between j-th hidden neuron and k-th output neuron is $w_{kj}^{(2)}$.



Neural Networks
Forward Propagation

- For input $\mathbf{x}$, denote output of hidden layer as the vector $\mathbf{z}(\mathbf{x}) \in \mathbb{R}^M$.
- Model $z_j(\mathbf{x})$ as a non-linear function $h(a_j)$ where *pre-activation* $a_j = \mathbf{w}_j^{(1)\,T}\mathbf{x}$ with adjustable parameters $\mathbf{w}_j^{(1)}$.



- So the k-th output can be written as

$$y_k(\mathbf{x}) = f(a_k) = f(\mathbf{w}_k^{(2)\,T}\mathbf{z}(\mathbf{x}))$$

$$= f\left(\sum_{j=1}^{M} w_{kj}^{(2)} z_j(\mathbf{x}) + w_{k0}^{(2)}\right) = f\left(\sum_{j=1}^{M} w_{kj}^{(2)} h\left(\sum_{i=0}^{D} w_{ji}^{(1)} x_i\right) + w_{k0}^{(2)}\right)$$

where we have prepended $x_0 = 1$ to to absorb bias input and $w_{j0}^{(1)}$ and $w_{k0}^{(2)}$ represent biases.

Neural Networks
Forward Propagation

- The computation

$$y_k(\mathbf{x}, \mathbf{W}) = f\left(\sum_{j=1}^{M} w_{kj}^{(2)} h\left(\sum_{i=0}^{D} w_{ji}^{(1)} x_i\right) + w_{k0}^{(2)}\right)$$

  can be viewed in two stages:
  1. $z_j = h(\mathbf{w}_j^{(1)\,T}\mathbf{x})$ for $j = 1, \ldots, M$.
  2. $y_k = f(\mathbf{w}_k^{(2)\,T}\mathbf{z})$.

Neural Networks
Forward Propagation

- If we define the matrices

$$\mathbf{W}^{(1)} = \underbrace{\begin{bmatrix} \longleftarrow & \mathbf{w}_1^{(1)\,T} & \longrightarrow \\ \longleftarrow & \mathbf{w}_2^{(1)\,T} & \longrightarrow \\ & \vdots & \\ \longleftarrow & \mathbf{w}_M^{(1)\,T} & \longrightarrow \end{bmatrix}}_{M\times(D+1)} \text{ and } \mathbf{W}^{(2)} = \underbrace{\begin{bmatrix} \longleftarrow & \mathbf{w}_1^{(2)\,T} & \longrightarrow \\ \longleftarrow & \mathbf{w}_2^{(2)\,T} & \longrightarrow \\ & \vdots & \\ \longleftarrow & \mathbf{w}_K^{(2)\,T} & \longrightarrow \end{bmatrix}}_{K\times(M+1)}$$

  then forward propagation constitutes
  1. $\mathbf{z} = h(\mathbf{W}^{(1)}\mathbf{x})$.
  2. Prepend 1 to $\mathbf{z}$.
  3. $\mathbf{y} = f(\mathbf{W}^{(2)}\mathbf{z})$.

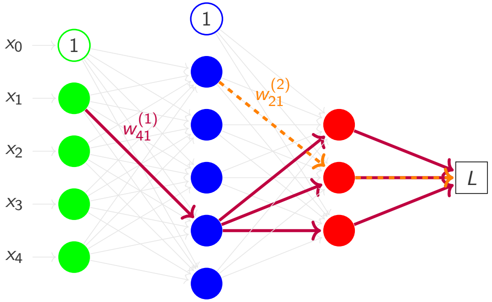
Neural Networks for Regression
Gradients

- Regression requires continuous output $y_k \in \mathbb{R}$.
- So use *identity* activation function $y_k = f(a_k) = a_k$.
- Loss can be written as

$$L(\mathbf{W}^{(1)}, \mathbf{W}^{(2)}) = \frac{1}{2} \sum_{n=1}^{N} \underbrace{\|\mathbf{y}_n - \mathbf{t}_n\|^2}_{L_n} = \frac{1}{2} \sum_{n=1}^{N} \sum_{k=1}^{K} (y_{nk} - t_{nk})^2$$

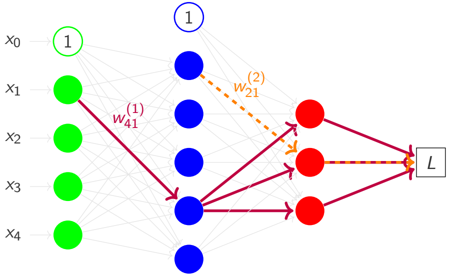
- Loss L depends on sum of individual losses L_n.
- In the following, we will focus on loss L_n for the n-th training sample.
- We will drop n for notational clarity and refer to L_n simply as L.

How do weights influence loss?



- $w_{kj}^{(2)}$ influences $a_k^{(2)}$ which influences y_k which influences L.
- For scalar dependencies, use chain rule.
- $w_{ji}^{(1)}$ influences $a_j^{(1)}$ which influences z_j which influences $a_1^{(2)}, a_2^{(2)}, a_3^{(2)}$ which influence y_1, y_2, y_3 which influence L.
- For vector/multivariate dependencies, use multivariate chain rule.

How do weights influence loss?



- Layer 2: $L \leftarrow y_k \leftarrow a_k^{(2)} \leftarrow w_{kj}^{(2)}$.

$$L(y_k(a_k^{(2)}(w_{kj}^{(2)})))$$

- Layer 1: $L \leftarrow \mathbf{y} \leftarrow \mathbf{a}^{(2)} \leftarrow z_j \leftarrow a_j^{(1)} \leftarrow w_{ji}^{(1)}$.

$$L(\underbrace{y_1(a_1^{(2)}(z_j(a_j^{(1)}(w_{ji}^{(1)}))))}_{y_1(w_{ji}^{(1)})}, \underbrace{y_2(a_2^{(2)}(z_j(a_j^{(1)}(w_{ji}^{(1)}))))}_{y_2(w_{ji}^{(1)})}, \dots, \underbrace{y_k(a_k^{(2)}(z_j(a_j^{(1)}(w_{ji}^{(1)}))))}_{y_k(w_{ji}^{(1)})})$$

Multivariate Chain Rule

- The chain rule of differentiation states

$$\frac{df(u(x))}{dx} = \frac{df}{du}\frac{du}{dx}$$

$$\begin{tikzcd} x \arrow[r] & u \arrow[r] & f \end{tikzcd}$$

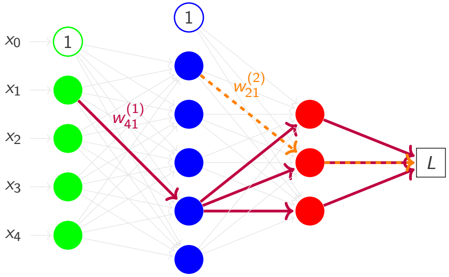
- The *multivariate* chain rule of differentiation states

$$\frac{df(u(x),v(x))}{dx} = \frac{\partial f}{\partial u}\frac{du}{dx} + \frac{\partial f}{\partial v}\frac{dv}{dx}$$

$$\begin{tikzcd} & u \arrow[dr] & \\ x \arrow[ur] \arrow[dr] & & f(u,v) \\ & v \arrow[ur] & \end{tikzcd}$$

- The multivariate chain rule applied to compute derivatives w.r.t weights of hidden layers has a special name – *backpropagation*.

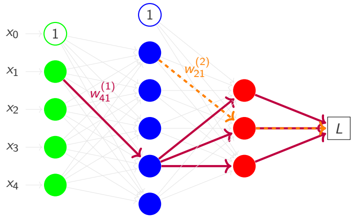
Backpropagation



- For the output layer weights

$$\frac{\partial L(y_k(a_k^{(2)}(w_{kj}^{(2)})))}{\partial w_{kj}^{(2)}} = \frac{\partial L}{\partial a_k^{(2)}} \frac{\partial a_k^{(2)}}{\partial w_{kj}^{(2)}} = \delta_k z_j$$

Backpropagation



- For the hidden layer weights, using the multivariate chain rule

$$\frac{\partial}{\partial w_{ji}^{(1)}} L(y_1(a_1^{(2)}(z_j(a_j^{(1)}(w_{ji}^{(1)})))), y_2(a_2^{(2)}(z_j(a_j^{(1)}(w_{ji}^{(1)})))), \ldots, y_k(a_k^{(2)}(z_j(a_j^{(1)}(w_{ji}^{(1)})))))$$

$$= \frac{\partial L}{\partial a_j^{(1)}} \frac{\partial a_j^{(1)}}{\partial w_{ji}^{(1)}} = \underbrace{\sum_{k=1}^{K} \underbrace{\frac{\partial L}{\partial a_k^{(2)}}}_{\delta_k} \underbrace{\frac{\partial a_k^{(2)}}{\partial z_j}}_{w_{kj}^{(2)}} \underbrace{\frac{\partial z_j}{\partial a_j^{(1)}}}_{h'(a_j^{(1)})}}_{\frac{\partial L}{\partial a_j^{(1)}} = \delta_j} \underbrace{\frac{\partial a_j^{(1)}}{\partial w_{ji}^{(1)}}}_{x_i} = \delta_j x_i$$

- Notice that gradient = $\delta \times$ input

Backpropagation

- It is important to note that

$$\delta_j = h'(a_j) \sum_{k=1}^{K} \delta_k w_{kj}$$

  yields the error δ_j at hidden neuron j by *backpropagating* the errors δ_k from all output neurons that use the output of neuron j.
- More generally, compute error δ_j at a layer by *backpropagating* the errors δ_k from next layer.
- Hence the names *error backpropagation*, *backpropagation*, or simply *backprop*.
- Very useful machine learning technique that is *not limited to neural networks*.

Backpropagation

$$\delta_j^{(1)} = h'(a_j) \sum_{k=1}^{K} \delta_k^{(2)} w_{kj}$$

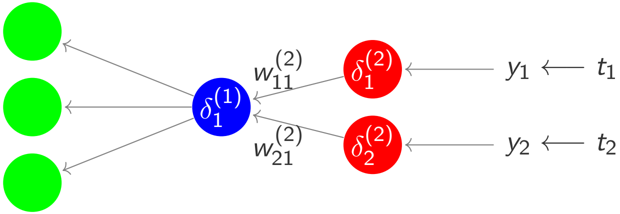


Figure: Visual representation of backpropagation of delta values of layer $l + 1$ to compute delta values of layer l.

Backpropagation
Learning Algorithm

1. Forward propagate the input vector $\mathbf{x}_n$ to compute *and store* activations and outputs of every neuron in every layer.
2. Evaluate $\delta_k = \frac{\partial L_n}{\partial a_k}$ for every neuron in output layer.
3. Evaluate $\delta_j = \frac{\partial L_n}{\partial a_j}$ for every neuron in *every* hidden layer via backpropagation.

$$\delta_j = h'(a_j) \sum_{k=1}^{K} \delta_k w_{kj}$$

4. Compute derivative of each weight $\frac{\partial L_n}{\partial w}$ via $\delta \times$input.
5. Update each weight via gradient descent $w^{\tau+1} = w^{\tau} - \eta \frac{\partial L_n}{\partial w}$.

Tanh
A $(-1,1)$ sigmoidal function

- Since range of logistic sigmoid $\sigma(a)$ is $(0,1)$, we can obtain a function with $(-1,1)$ range as $2\sigma(a)-1$.
- Another related function with $(-1,1)$ range is the tanh function.

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

  where σ is applied on $2a$.
- Preferred[1]over logistic sigmoid as activation function $h(a)$ of hidden neurons.
- Just like the logistic sigmoid, derivative of $\tanh(a)$ is simple: $1-\tanh^2(a)$. (Prove it.)

[1]LeCun et al., ‘Efficient backprop’.

A Simple Example

- Two-layer MLP for multivariate regression from $\mathbb{R}^D \longrightarrow \mathbb{R}^K$.
- Linear outputs $y_k = a_k$ with half-SSE $L = \frac{1}{2}\sum_{k=1}^{K}(y_k - t_k)^2$.
- M hidden neurons with $\tanh(\cdot)$ activation functions.

Forward propagation

$$a_j = \sum_{i=0}^{D} w_{ji}^{(1)} x_i$$

$$z_j = \tanh(a_j)$$

$$z_0 = 1$$

$$y_k = \sum_{j=0}^{M} w_{kj}^{(2)} z_j$$

$$\delta_k = y_k - t_k$$

Backpropagation

$$\delta_j = (1 - z_j^2)\sum_{k=1}^{K} w_{kj}^{(2)} \delta_k$$

- Compute derivatives $\frac{\partial L}{\partial w_{ji}^{(1)}} = \delta_j x_i$ and $\frac{\partial L}{\partial w_{kj}^{(2)}} = \delta_k z_j$.

Backpropagation
Verifying Correctness

- *Numerical derivatives* can be computed via finite *central differences*

$$\frac{\partial L_n}{\partial w_{ji}} = \frac{L_n(w_{ji}+\epsilon) - L_n(w_{ji}-\epsilon)}{2\epsilon} + O(\epsilon^2)$$

- *Analytical derivatives* computed via backpropagation **must be compared** with numerical derivatives for a few examples to verify correctness.
- Any implementation of analytical derivatives (not just backpropagation) must be compared with numerical derivatives.
- Notice that we could have avoided backpropagation and computed all required derivatives numerically.
  - But cost of numerical differentiation is $O(W^2)$ while that of backpropagation is $O(W)$ where W is the total number of weights (and biases) in the network. (Why?)

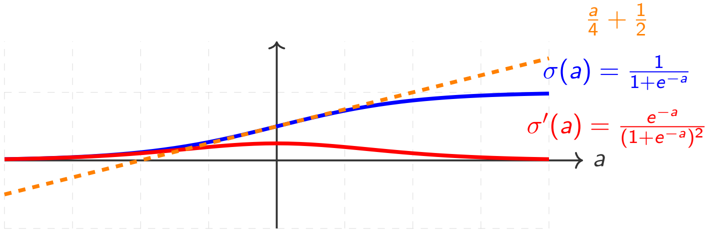
Neural Network training finds local minimum

- For optimisation, we notice that $\mathbf{w}^*$ must be a *stationary point* of $E(\mathbf{w})$.
  - Minimum, maximum, or saddle point.
  - A saddle point is where gradient vanishes but point is not an extremum (Example).
- The goal in neural network minimisation is to find a local minimum.
- A global minimum, *even if found*, cannot be verified as globally minimum.
- Due to symmetry, there are multiple equivalent local minima. Reaching *any suitable* local minimum is the goal of neural network optimisation.
- Since there are no analytical solutions for $\mathbf{w}^*$, we use iterative, numerical procedures.

Optimisation Options

- Options for iterative optimisation
  - Online methods
    - Stochastic gradient descent
    - Stochastic gradient descent using mini-batches
  - Batch methods
    - Batch gradient descent
    - Conjugate gradient descent
    - Quasi-Newton methods
- Online methods
  - converge faster since parameter updates are more frequent, and
  - have greater chance of escaping local minima because stationary point w.r.t to whole data set will generally not be a stationary point w.r.t an individual data point.
- Batch methods: Conjugate gradient descent and quasi-Newton methods
  - are more robust and faster than batch gradient descent, and
  - decrease the error function at each iteration until arriving at a minimum.

Problems with sigmoidal neurons



- For large $|a|$, sigmoid value approaches either 0 or 1. This is called *saturation*.
- When the sigmoid saturates, the gradient approaches zero.
- Neurons with sigmoidal activations stop learning when they saturate.
- When they are not saturated, they are almost linear.
- There is another reason for the gradient to approach zero during backpropagation.

Vanishing Gradients

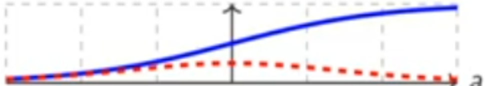
- Notice that gradient of the sigmoid is always between 0 and $\frac{1}{4}$.
- Now consider the backpropagation equation.

$$\delta_j = \underbrace{h'(a_j)}_{\leq \frac{1}{4}} \sum_{k=1}^{K} w_{kj}\delta_k$$

where $\underline{\delta_k \text{ will also contain } \textit{at least} \text{ one factor of } \leq \frac{1}{4}}$.

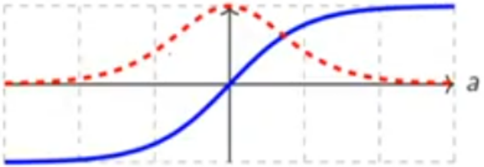
- This means that values of δ_j keep getting smaller as we backpropagate towards the early layers.
- Since gradient $= \delta \times$input, the gradients also keep getting smaller for the earlier layers. Known as the *vanishing gradients* problem.
- *Therefore, while the network might be deep, learning will not be deep.*

Logistic Sigmoid



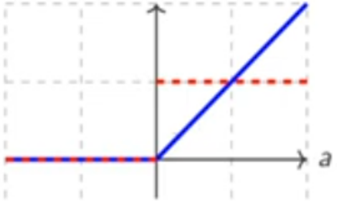
Activation function	$y(a) = \frac{1}{1+e^{-a}}$
Derivative	$y'(a) = y(a)(1 - y(a))$
Maximum magnitude of derivative	$\frac{1}{4}$
Problem	Cause vanishing gradients

Hyperbolic Tangent



Activation function	$y(a) = \tanh(a)$
Derivative	$y'(a) = 1 - y^2(a)$
Maximum magnitude of derivative	1
Problem	Cause vanishing gradients

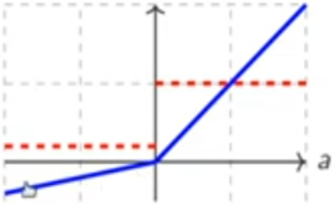
Rectified Linear Unit (ReLU)



Activation function	$y(a) = \begin{cases} a & \text{if } a > 0 \\ 0 & \text{if } a \leq 0 \end{cases}$
Derivative	$y'(a) = \begin{cases} 1 & \text{if } a > 0 \\ 0 & \text{if } a \leq 0 \end{cases}$
Advantage	Avoids vanishing gradients
Problem	Dead neurons[2]

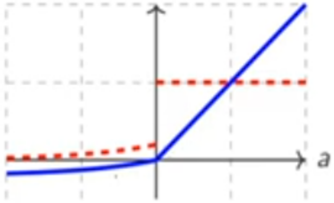
[2] This can be an advantage as well since death implies fewer neurons.

Leaky ReLU



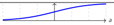
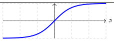
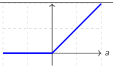
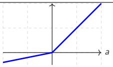
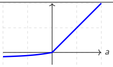
Activation function	$y(a) = \begin{cases} a & \text{if } a > 0 \\ ka & \text{if } a \leq 0 \end{cases}$ where $0 \leq k \leq 1$
Derivative	$y'(a) = \begin{cases} 1 & \text{if } a > 0 \\ k & \text{if } a \leq 0 \end{cases}$
Advantage	Neuron is always learning

Exponential Linear Unit (ELU)



Activation function	$y(a) = \begin{cases} a & \text{if } a > 0 \\ k(e^a - 1) & \text{if } a \leq 0 \end{cases}$ where $k > 0$
Derivative	$y'(a) = \begin{cases} 1 & \text{if } a > 0 \\ y(a) + k & \text{if } a \leq 0 \end{cases}$
Maximum magnitude of derivative	1
Advantage	Neuron is mostly learning

Better Activation Functions

Name	f(a)	Plot	Derivative	Comments
Logistic sigmoid	$\frac{1}{1+e^{-a}}$		$f(a)(1-f(a))$	Vanishing gradients
Hyperbolic tangent	$\tanh(a)$		$1-\tanh^2(a)$	Vanishing gradients
Rectified Linear Unit (ReLU)	$\begin{cases} a & \text{if } a>0 \\ 0 & \text{if } a \le 0 \end{cases}$		$\begin{cases} 1 \\ 0 \end{cases}$	Dead neurons. Sparsity.
Leaky ReLU	$\begin{cases} a & \text{if } a>0 \\ ka & \text{if } a \le 0 \end{cases}$		$\begin{cases} 1 \\ k \end{cases}$	$0<k<1$
Exponential Linear Unit (ELU)	$\begin{cases} a & \text{if } a>0 \\ k(e^a-1) & \text{if } a \le 0 \end{cases}$		$\begin{cases} 1 \\ f(a)-k \end{cases}$	$k>0$.

- Saturated sigmoidal neurons stop learning. Piecewise-linear units keep learning by avoiding saturation.
- ELU leads to better accuracy and faster training.
- *Take home message*: For hidden neurons, use a member of the LU family. They avoid *i*) saturation and *ii*) the vanishing gradient problem.