EC-332 Machine Learning

Backpropagation and Vanishing Gradients

Nazar Khan
Department of Computer Science
University of the Punjab

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] **lecun1998efficient**.

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

- Any implementation of analytical derivatives (not just backpropagation) must be compared with numerical derivatives.
- *Numerical derivatives* can be computed via finite *central differences*

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

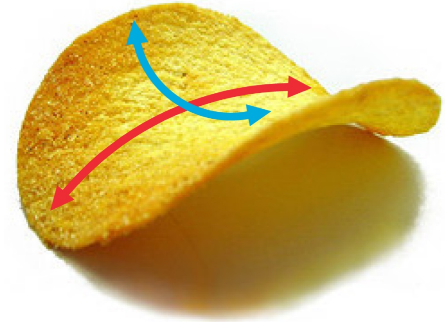
- *Analytical derivatives* computed via backpropagation **must be compared** with numerical derivatives for a few examples to verify correctness.

Backpropagation
Efficiency

- Notice that we could have avoided backpropagation and computed all required derivatives numerically.
- But cost of numerical differentiation is $O(|W|^2)$.
  - Two fprops per weight and each fprop has $O(|W|)$ cost. Why?
- While cost of backpropagation is $O(|W|)$.

Neural Networks and Stationary Points

- For optimisation, we notice that W^* must be a *stationary point* of $L(W)$.
  - Minimum, maximum, or saddle point.
  - A saddle point is where gradient vanishes but point is not an extremum.



Neural Network training finds local minimum

- 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 W^*, we use iterative, numerical procedures.

Optimisation Options

- Options for iterative optimisation
  - Online methods (using partial training data)
    - Stochastic gradient descent
    - Stochastic gradient descent using mini-batches
  - Batch methods (using all training data)
    - Batch gradient descent
    - Conjugate gradient descent
    - Quasi-Newton methods

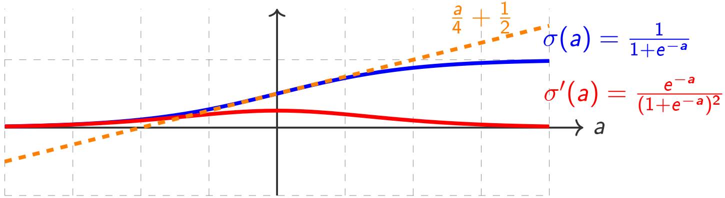
Online Methods

- Online methods converge faster since parameter updates are more frequent.
- 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

- Batch methods are practical for small datasets only.
- Deep Learning datasets are increasingly becoming larger and larger.
- Conjugate gradient descent and quasi-Newton methods
  - are more robust and faster than batch gradient descent, and
  - decrease loss 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 Gradient

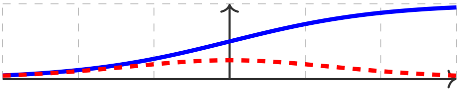
- Notice that gradient of the sigmoid is always between 0 and $\frac{1}{4}$.
- Now consider the backpropagation equation.

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

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

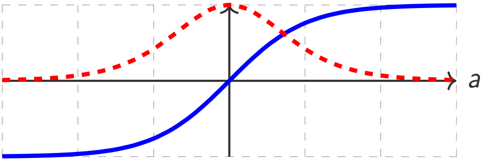
- This means that values of δ_j keep getting smaller as we backpropagate towards the early layers.
- Since gradient $= \delta \times$input, the gradients also keep getting smaller for the earlier layers. Known as the *vanishing gradient* problem.
- *Therefore, while the network might be deep, learning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

Logistic Sigmoid



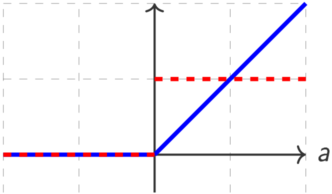
Activation function	$y(a) = \frac{1}{1+e^{-a}}$
Derivative	$y'(a) = y(a)(1 - y(a))$
Maximum magnitude of derivative	$\frac{1}{4}$
Problem	Cause vanishing gradients

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 $y(a) = \begin{cases} a & \text{if } a > 0 \\ 0 & \text{if } a \leq 0 \end{cases}$

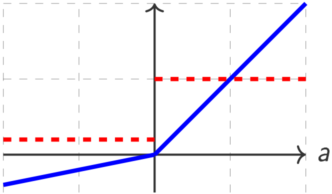
Derivative $y'(a) = \begin{cases} 1 & \text{if } a > 0 \\ 0 & \text{if } a \leq 0 \end{cases}$

Advantage Avoids vanishing gradients

Problem Dead neurons[2]

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

Leaky ReLU



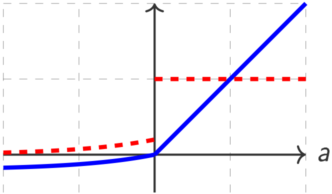
Activation function $y(a) = \begin{cases} a & \text{if } a > 0 \\ ka & \text{if } a \leq 0 \end{cases}$

where $0 \leq k \leq 1$

Derivative $y'(a) = \begin{cases} 1 & \text{if } a > 0 \\ k & \text{if } a \leq 0 \end{cases}$

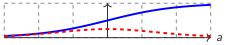
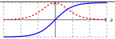
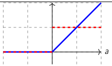
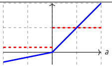
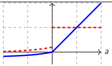
Advantage Neuron is always learning

Exponential Linear Unit (ELU)



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

Activation Functions
Summary

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

- Saturated sigmoidal neurons stop learning. Piecewise-linear units keep learning by avoiding saturation.
- ELU has been shown to lead 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.