January 29-February 2 : Advanced machine learning and data analysis for the physical sciences

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January 30

Overview of third week

1. Discussion of possible projects
2. Review of neural networks and automatic differentiation
3. Discussion of codes

Mathematics of deep learning

Two recent books online.

1. The Modern Mathematics of Deep Learning, by Julius Berner, Philipp Grohs, Gitta Kutyniok, Philipp Petersen, published as Mathematical Aspects of Deep Learning, pp. 1-111. Cambridge University Press, 2022
2. Mathematical Introduction to Deep Learning: Methods, Implementations, and Theory, Arnulf Jentzen, Benno Kuckuck, Philippe von Wurstemberger

Reminder on books with hands-on material and codes

- Sebastian Rashcka et al, Machine learning with Sickit-Learn and PyTorch
- David Foster, Generative Deep Learning with TensorFlow

- Bali and Gavras, Generative AI with Python and TensorFlow 2

All three books have GitHub addresses from where one can download all codes. We will borrow most of the material from these three texts as well as from Goodfellow, Bengio and Courville's text Deep Learning

Reading recommendations

1. Rashkca et al., chapter 11, jupyter-notebook sent separately, from GitHub
2. Goodfellow et al, chapter 6 and 7 contain most of the neural network background.

Mathematics of deep learning and neural networks

Neural networks, in its so-called feed-forward form, where each iterations contains a feed-forward stage and a back-propgagation stage, consist of series of affine matrix-matrix and matrix-vector multiplications. The unknown parameters (the so-called biases and weights which deternine the architecture of a neural network), are uptaded iteratively using the so-called back-propagation algorithm. This algorithm corresponds to the so-called reverse mode of automatic differentation.

Basics of an NN

A neural network consists of a series of hidden layers, in addition to the input and output layers. Each layer l has a set of parameters $\boldsymbol{\Theta}^{(l)} = (\boldsymbol{W}^{(l)}, \boldsymbol{b}^{(l)})$ which are related to the parameters in other layers through a series of affine transformations, for a standard NN these are matrix-matrix and matrix-vector multiplications. For all layers we will simply use a collective variable $\boldsymbol{\Theta}$.

It consist of two basic steps:

1. a feed forward stage which takes a given input and produces a final output which is compared with the target values through our cost/loss function.
2. a back-propagation state where the unknown parameters $\boldsymbol{\Theta}$ are updated through the optimization of the their gradients. The expressions for the gradients are obtained via the chain rule, starting from the derivative of the cost/function.

These two steps make up one iteration. This iterative process is continued till we reach an eventual stopping criterion.

Overarching view of a neural network

The architecture of a neural network defines our model. This model aims at describing some function $f(\boldsymbol{x}$ which represents some final result (outputs or tagrget values) given a specific inpput $\boldsymbol{x}$. Note that here $\boldsymbol{y}$ and $\boldsymbol{x}$ are not limited to be vectors.

The architecture consists of

1. An input and an output layer where the input layer is defined by the inputs $\boldsymbol{x}$. The output layer produces the model ouput $\tilde{\boldsymbol{y}}$ which is compared with the target value $\boldsymbol{y}$
2. A given number of hidden layers and neurons/nodes/units for each layer (this may vary)
3. A given activation function $\sigma(\boldsymbol{z})$ with arguments $\boldsymbol{z}$ to be defined below. The activation functions may differ from layer to layer.
4. The last layer, normally called **output** layer has normally an activation function tailored to the specific problem
5. Finally we define a so-called cost or loss function which is used to gauge the quality of our model.

The optimization problem

The cost function is a function of the unknown parameters $\boldsymbol{\Theta}$ where the latter is a container for all possible parameters needed to define a neural network

If we are dealing with a regression task a typical cost/loss function is the mean squared error

$$C(\boldsymbol{\Theta}) = \frac{1}{n}\left\{\left(\boldsymbol{y}-\boldsymbol{X}\boldsymbol{\theta}\right)^T\left(\boldsymbol{y}-\boldsymbol{X}\boldsymbol{\theta}\right)\right\}.$$

This function represents one of many possible ways to define the so-called cost function. Note that here we have assumed a linear dependence in terms of the paramters $\boldsymbol{\Theta}$. This is in general not the case.

Parameters of neural networks

For neural networks the parameters $\boldsymbol{\Theta}$ are given by the so-called weights and biases (to be defined below).

The weights are given by matrix elements $w_{ij}^{(l)}$ where the superscript indicates the layer number. The biases are typically given by vector elements representing each single node of a given layer, that is $b_j^{(l)}$.

Other ingredients of a neural network

Having defined the architecture of a neural network, the optimization of the cost function with respect to the parameters $\boldsymbol{\Theta}$, involves the calculations of gradients and their optimization. The gradients represent the derivatives of a multidimensional object and are often approximated by various gradient methods, including

1. various quasi-Newton methods,

2. plain gradient descent (GD) with a constant learning rate η,
3. GD with momentum and other approximations to the learning rates such as
   - Adapative gradient (ADAgrad)
   - Root mean-square propagation (RMSprop)
   - Adaptive gradient with momentum (ADAM) and many other
4. Stochastic gradient descent and various families of learning rate approximations

Other parameters

In addition to the above, there are often additional hyperparamaters which are included in the setup of a neural network. These will be discussed below.

Universal approximation theorem

The universal approximation theorem plays a central role in deep learning. Cybenko (1989) showed the following:

Let σ be any continuous sigmoidal function such that

$$\sigma(z) = \left\{\begin{array}{cc} 1 & z\rightarrow \infty\\ 0 & z \rightarrow -\infty \end{array}\right.$$

Given a continuous and deterministic function $F(\boldsymbol{x})$ on the unit cube in d-dimensions $F\in [0,1]^d$, $x\in [0,1]^d$ and a parameter $\epsilon > 0$, there is a one-layer (hidden) neural network $f(\boldsymbol{x};\boldsymbol{\Theta})$ with $\boldsymbol{\Theta}=(\boldsymbol{W},\boldsymbol{b})$ and $\boldsymbol{W}\in \mathbb{R}^{m\times n}$ and $\boldsymbol{b}\in \mathbb{R}^{n}$, for which

$$\vert F(\boldsymbol{x})-f(\boldsymbol{x};\boldsymbol{\Theta})\vert < \epsilon \hspace{0.1cm} \forall \boldsymbol{x}\in[0,1]^d.$$

Some parallels from real analysis

For those of you familiar with for example the Stone-Weierstrass theorem for polynomial approximations or the convergence criterion for Fourier series, there are similarities in the derivation of the proof for neural networks. See whiteboard notes for week 2.

The approximation theorem in words

Any continuous function $y = F(\boldsymbol{x})$ supported on the unit cube in d-dimensions can be approximated by a one-layer sigmoidal network to arbitrary accuracy.

Hornik (1991) extended the theorem by letting any non-constant, bounded activation function to be included using that the expectation value

$$\mathbb{E}[|F(\boldsymbol{x})|^2] = \int_{\boldsymbol{x}\in D} |F(\boldsymbol{x})|^2 p(\boldsymbol{x}) d\boldsymbol{x} < \infty.$$

Then we have

$$\mathbb{E}[|F(\boldsymbol{x}) - f(\boldsymbol{x};\boldsymbol{\Theta})|^2] = \int_{\boldsymbol{x}\in D} |F(\boldsymbol{x}) - f(\boldsymbol{x};\boldsymbol{\Theta})|^2 p(\boldsymbol{x}) d\boldsymbol{x} < \epsilon.$$

More on the general approximation theorem

None of the proofs give any insight into the relation between the number of of hidden layers and nodes and the approximation error ϵ, nor the magnitudes of $\boldsymbol{W}$ and $\boldsymbol{b}$.

Neural networks (NNs) have what we may call a kind of universality no matter what function we want to compute.

It does not mean that an NN can be used to exactly compute any function. Rather, we get an approximation that is as good as we want.

Class of functions we can approximate

The class of functions that can be approximated are the continuous ones. If the function $F(\boldsymbol{x})$ is discontinuous, it won't in general be possible to approximate it. However, an NN may still give an approximation even if we fail in some points.

Setting up the equations for a neural network

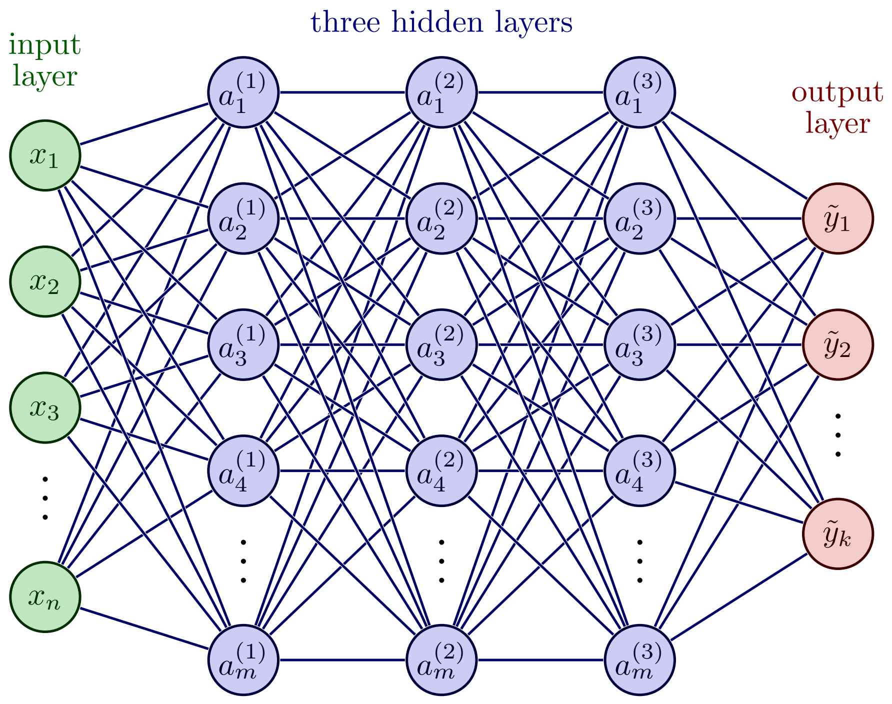
The questions we want to ask are how do changes in the biases and the weights in our network change the cost function and how can we use the final output to modify the weights and biases?

To derive these equations let us start with a plain regression problem and define our cost function as

$$\mathcal{C}(\boldsymbol{\Theta}) = \frac{1}{2}\sum_{i=1}^{n} \left(y_i - \tilde{y}_i\right)^2,$$

where the y_is are our n targets (the values we want to reproduce), while the outputs of the network after having propagated all inputs $\boldsymbol{x}$ are given by $\boldsymbol{\tilde{y}}_i$.

Layout of a neural network with three hidden layers



Definitions

With our definition of the targets $\boldsymbol{y}$, the outputs of the network $\tilde{\boldsymbol{y}}$ and the inputs $\boldsymbol{x}$ we define now the activation z_j^l of node/neuron/unit j of the l-th layer as a function of the bias, the weights which add up from the previous layer $l-1$ and the forward passes/outputs $\hat{a}^{l-1}$ from the previous layer as

$$z_j^l = \sum_{i=1}^{M_{l-1}} w_{ij}^l a_i^{l-1} + b_j^l,$$

where b_k^l are the biases from layer l. Here M_{l-1} represents the total number of nodes/neurons/units of layer $l-1$. The figure in the whiteboard notes illustrates this equation. We can rewrite this in a more compact form as the matrix-vector products we discussed earlier,

$$\hat{z}^l = \left(\hat{W}^l\right)^T \hat{a}^{l-1} + \hat{b}^l.$$

Inputs to the activation function

With the activation values $\boldsymbol{z}^l$ we can in turn define the output of layer l as $\boldsymbol{a}^l = f(\boldsymbol{z}^l)$ where f is our activation function. In the examples here we will use the sigmoid function discussed in our logistic regression lectures. We will also use the same activation function f for all layers and their nodes. It means we have

$$a_j^l = \sigma(z_j^l) = \frac{1}{1+\exp -(z_j^l)}.$$

Derivatives and the chain rule

From the definition of the activation z_j^l we have

$$\frac{\partial z_j^l}{\partial w_{ij}^l} = a_i^{l-1},$$

and

$$\frac{\partial z_j^l}{\partial a_i^{l-1}} = w_{ji}^l.$$

With our definition of the activation function we have that (note that this function depends only on z_j^l)

$$\frac{\partial a_j^l}{\partial z_j^l} = a_j^l(1-a_j^l) = \sigma(z_j^l)(1-\sigma(z_j^l)).$$

Derivative of the cost function

With these definitions we can now compute the derivative of the cost function in terms of the weights.

Let us specialize to the output layer $l = L$. Our cost function is

$$\mathcal{C}(\boldsymbol{\Theta}^L) = \frac{1}{2}\sum_{i=1}^{n}(y_i - \tilde{y}_i)^2 = \frac{1}{2}\sum_{i=1}^{n}\left(a_i^L - y_i\right)^2,$$

The derivative of this function with respect to the weights is

$$\frac{\partial \mathcal{C}(\boldsymbol{\Theta}^L)}{\partial w_{jk}^L} = \left(a_j^L - y_j\right)\frac{\partial a_j^L}{\partial w_{jk}^L},$$

The last partial derivative can easily be computed and reads (by applying the chain rule)

$$\frac{\partial a_j^L}{\partial w_{jk}^L} = \frac{\partial a_j^L}{\partial z_j^L}\frac{\partial z_j^L}{\partial w_{jk}^L} = a_j^L(1-a_j^L)a_k^{L-1}.$$

Simpler examples first and automatic differentiation

In order to understand the back propagation algorithm and its derivation (an implementation of the chain rule), let us first digress with some simple examples. These examples are also meant to motivate the link with back propagation and automatic differentiation.

Reminder on the chain rule and gradients

If we have a multivariate function $f(x,y)$ where $x = x(t)$ and $y = y(t)$ are functions of a variable t, we have that the gradient of f with respect to t (without the explicit unit vector components)

$$\frac{df}{dt} = \begin{bmatrix} \frac{\partial f}{\partial x} & \frac{\partial f}{\partial y} \end{bmatrix} \begin{bmatrix} \frac{\partial x}{\partial t} \\ \frac{\partial y}{\partial t} \end{bmatrix} = \frac{\partial f}{\partial x}\frac{\partial x}{\partial t} + \frac{\partial f}{\partial y}\frac{\partial y}{\partial t}.$$

Multivariable functions

If we have a multivariate function $f(x,y)$ where $x = x(t,s)$ and $y = y(t,s)$ are functions of the variables t and s, we have that the partial derivatives

$$\frac{\partial f}{\partial s} = \frac{\partial f}{\partial x}\frac{\partial x}{\partial s} + \frac{\partial f}{\partial y}\frac{\partial y}{\partial s},$$

and

$$\frac{\partial f}{\partial t} = \frac{\partial f}{\partial x}\frac{\partial x}{\partial t} + \frac{\partial f}{\partial y}\frac{\partial y}{\partial t}.$$

the gradient of f with respect to t and s (without the explicit unit vector components)

$$\frac{df}{d(s,t)} = \begin{bmatrix} \frac{\partial f}{\partial x} & \frac{\partial f}{\partial y} \end{bmatrix} \begin{bmatrix} \frac{\partial x}{\partial s} & \frac{\partial x}{\partial t} \\ \frac{\partial x}{\partial s} & \frac{\partial y}{\partial t} \end{bmatrix}.$$

Automatic differentiation through examples

A great introduction to automatic differentiation is given by Baydin et al., see `https://arxiv.org/abs/1502.05767`.

Automatic differentiation is a represented by a repeated application of the chain rule on well-known functions and allows for the calculation of derivatives to numerical precision. It is not the same as the calculation of symbolic derivatives via for example SymPy, nor does it use approximative formulae based on Taylor-expansions of a function around a given value. The latter are error prone due to truncation errors and values of the step size Δ.

Simple example

Our first example is rather simple,

$$f(x) \exp x^2,$$

with derivative

$$f'(x)2x\exp x^2.$$

We can use SymPy to extract the pertinent lines of Python code through the following simple example

```
from __future__ import division
from sympy import *
x = symbols('x')
expr = sqrt(x*x+exp(x*x))
simplify(expr)
derivative = diff(expr,x)
print(python(expr))
print(python(derivative))
```

Smarter way of evaluating the above function

If we study this function, we note that we can reduce the number of operations by introducing an intermediate variable

$$a = x^2,$$

leading to

$$f(x) = f(a(x)) = b = \exp a.$$

We now assume that all operations can be counted in terms of equal floating point operations. This means that in order to calculate $f(x)$ we need first to square x and the compute the exponential. We have thus two floating point operations only.

Reducing the number of operations

With the introduction of a precalculated quantity a and thereby $f(x)$ we have that the derivative can be written as

$$f'(x) = 2xb,$$

which reduces the number of operations from four in the orginal expression to two. This means that if we need to compute $f(x)$ and its derivative (a common task in optimizations), we have reduced the number of operations from six to four in total.

Note that the usage of a symbolic software like SymPy does not include such simplifications and the calculations of the function and the derivatives yield in general more floating point operations.

Chain rule, forward and reverse modes

In the above example we have introduced the variables a and b, and our function is

$$f(x) = f(a(x)) = b = \exp a,$$

with $a = x^2$. We can decompose the derivative of f with respect to x as

$$\frac{df}{dx} = \frac{df}{db}\frac{db}{da}\frac{da}{dx}.$$

We note that since $b = f(x)$ that

$$\frac{df}{db} = 1,$$

leading to

$$\frac{df}{dx} = \frac{db}{da}\frac{da}{dx} = \exp x^2,$$

as before.

First back propagation equation

We have thus

$$\frac{\partial \mathcal{C}((\boldsymbol{\Theta}^L)}{\partial w_{jk}^L} = \left(a_j^L - y_j\right) a_j^L(1-a_j^L)a_k^{L-1},$$

Defining

$$\delta_j^L = a_j^L(1-a_j^L)\left(a_j^L - y_j\right) = \sigma'(z_j^L)\frac{\partial \mathcal{C}}{\partial (a_j^L)},$$

and using the Hadamard product of two vectors we can write this as

$$\boldsymbol{\delta}^L = \sigma'(\hat{z}^L) \circ \frac{\partial \mathcal{C}}{\partial (\boldsymbol{a}^L)}.$$

Analyzing the last results

This is an important expression. The second term on the right handside measures how fast the cost function is changing as a function of the jth output activation. If, for example, the cost function doesn't depend much on a particular output node j, then δ_j^L will be small, which is what we would expect. The first term on the right, measures how fast the activation function f is changing at a given activation value z_j^L.

More considerations

Notice that everything in the above equations is easily computed. In particular, we compute z_j^L while computing the behaviour of the network, and it is only a small additional overhead to compute $\sigma'(z_j^L)$. The exact form of the derivative with respect to the output depends on the form of the cost function. However, provided the cost function is known there should be little trouble in calculating

$$\frac{\partial \mathcal{C}}{\partial (a_j^L)}$$

With the definition of δ_j^L we have a more compact definition of the derivative of the cost function in terms of the weights, namely

$$\frac{\partial \mathcal{C}}{\partial w_{jk}^L} = \delta_j^L a_k^{L-1}.$$

Derivatives in terms of z_j^L

It is also easy to see that our previous equation can be written as

$$\delta_j^L = \frac{\partial \mathcal{C}}{\partial z_j^L} = \frac{\partial \mathcal{C}}{\partial a_j^L}\frac{\partial a_j^L}{\partial z_j^L},$$

which can also be interpreted as the partial derivative of the cost function with respect to the biases b_j^L, namely

$$\delta_j^L = \frac{\partial \mathcal{C}}{\partial b_j^L}\frac{\partial b_j^L}{\partial z_j^L} = \frac{\partial \mathcal{C}}{\partial b_j^L},$$

That is, the error δ_j^L is exactly equal to the rate of change of the cost function as a function of the bias.

Bringing it together

We have now three equations that are essential for the computations of the derivatives of the cost function at the output layer. These equations are needed to start the algorithm and they are

$$\frac{\partial \mathcal{C}(\hat{W}^L)}{\partial w_{jk}^L} = \delta_j^L a_k^{L-1}, \tag{1}$$

and

$$\delta_j^L = \sigma'(z_j^L)\frac{\partial \mathcal{C}}{\partial (a_j^L)}, \tag{2}$$

and

$$\delta_j^L = \frac{\partial \mathcal{C}}{\partial b_j^L}, \tag{3}$$

Final back propagating equation

We have that (replacing L with a general layer l)

$$\delta_j^l = \frac{\partial \mathcal{C}}{\partial z_j^l}.$$

We want to express this in terms of the equations for layer $l+1$.

Using the chain rule and summing over all k entries

We obtain

$$\delta_j^l = \sum_k \frac{\partial \mathcal{C}}{\partial z_k^{l+1}} \frac{\partial z_k^{l+1}}{\partial z_j^l} = \sum_k \delta_k^{l+1} \frac{\partial z_k^{l+1}}{\partial z_j^l},$$

and recalling that

$$z_j^{l+1} = \sum_{i=1}^{M_l} w_{ij}^{l+1} a_i^l + b_j^{l+1},$$

with M_l being the number of nodes in layer l, we obtain

$$\delta_j^l = \sum_k \delta_k^{l+1} w_{kj}^{l+1} \sigma'(z_j^l),$$

This is our final equation.

We are now ready to set up the algorithm for back propagation and learning the weights and biases.

Setting up the back propagation algorithm

The four equations provide us with a way of computing the gradient of the cost function. Let us write this out in the form of an algorithm.

First, we set up the input data $\hat{x}$ and the activations $\hat{z}_1$ of the input layer and compute the activation function and the pertinent outputs $\hat{a}^1$.

Secondly, we perform then the feed forward till we reach the output layer and compute all $\hat{z}_l$ of the input layer and compute the activation function and the pertinent outputs $\hat{a}^l$ for $l = 1, 2, 3, \dots, L$.

Notation: The first hidden layer has $l = 1$ as label and the final output layer has $l = L$.

Setting up the back propagation algorithm, part 2

Thereafter we compute the ouput error $\hat{\delta}^L$ by computing all

$$\delta_j^L = \sigma'(z_j^L) \frac{\partial \mathcal{C}}{\partial (a_j^L)}.$$

Then we compute the back propagate error for each $l = L-1, L-2, \dots, 1$ as

$$\delta_j^l = \sum_k \delta_k^{l+1} w_{kj}^{l+1} \sigma'(z_j^l).$$

Setting up the Back propagation algorithm, part 3

Finally, we update the weights and the biases using gradient descent for each $l = L-1, L-2, \dots, 1$ and update the weights and biases according to the rules

$$w_{jk}^l \leftarrow= w_{jk}^l - \eta \delta_j^l a_k^{l-1},$$

$$b_j^l \leftarrow b_j^l - \eta \frac{\partial \mathcal{C}}{\partial b_j^l} = b_j^l - \eta \delta_j^l,$$

with η being the learning rate.

Updating the gradients

With the back propagate error for each $l = L-1, L-2, \dots, 1$ as

$$\delta_j^l = \sum_k \delta_k^{l+1} w_{kj}^{l+1} sigma'(z_j^l),$$

we update the weights and the biases using gradient descent for each $l = L-1, L-2, \dots, 1$ and update the weights and biases according to the rules

$$w_{jk}^l \leftarrow = w_{jk}^l - \eta \delta_j^l a_k^{l-1},$$

$$b_j^l \leftarrow b_j^l - \eta \frac{\partial \mathcal{C}}{\partial b_j^l} = b_j^l - \eta \delta_j^l,$$

Fine-tuning neural network hyperparameters

The flexibility of neural networks is also one of their main drawbacks: there are many hyperparameters to tweak. Not only can you use any imaginable network topology (how neurons/nodes are interconnected), but even in a simple FFNN you can change the number of layers, the number of neurons per layer, the type of activation function to use in each layer, the weight initialization logic, the stochastic gradient optmized and much more. How do you know what combination of hyperparameters is the best for your task?

- You can use grid search with cross-validation to find the right hyperparameters.

However,since there are many hyperparameters to tune, and since training a neural network on a large dataset takes a lot of time, you will only be able to explore a tiny part of the hyperparameter space.

- You can use randomized search.
- Or use tools like Oscar, which implements more complex algorithms to help you find a good set of hyperparameters quickly.

Hidden layers

For many problems you can start with just one or two hidden layers and it will work just fine. For the MNIST data set you ca easily get a high accuracy using just one hidden layer with a few hundred neurons. You can reach for this data set above 98% accuracy using two hidden layers with the same total amount of neurons, in roughly the same amount of training time.

For more complex problems, you can gradually ramp up the number of hidden layers, until you start overfitting the training set. Very complex tasks, such as large image classification or speech recognition, typically require networks with dozens of layers and they need a huge amount of training data. However, you will rarely have to train such networks from scratch: it is much more common to reuse parts of a pretrained state-of-the-art network that performs a similar task.

Which activation function should I use?

The Back propagation algorithm we derived above works by going from the output layer to the input layer, propagating the error gradient on the way. Once the algorithm has computed the gradient of the cost function with regards to each parameter in the network, it uses these gradients to update each parameter with a Gradient Descent (GD) step.

Unfortunately for us, the gradients often get smaller and smaller as the algorithm progresses down to the first hidden layers. As a result, the GD update leaves the lower layer connection weights virtually unchanged, and training never converges to a good solution. This is known in the literature as **the vanishing gradients problem**.

In other cases, the opposite can happen, namely the the gradients can grow bigger and bigger. The result is that many of the layers get large updates of the weights the algorithm diverges. This is the **exploding gradients problem**, which is mostly encountered in recurrent neural networks. More generally, deep neural networks suffer from unstable gradients, different layers may learn at widely different speeds

Is the Logistic activation function (Sigmoid) our choice?

Although this unfortunate behavior has been empirically observed for quite a while (it was one of the reasons why deep neural networks were mostly abandoned for a long time), it is only around 2010 that significant progress was made in understanding it.

A paper titled Understanding the Difficulty of Training Deep Feedforward Neural Networks by Xavier Glorot and Yoshua Bengio found that the problems with the popular logistic sigmoid activation function and the weight initialization technique that was most popular at the time, namely random initialization using a normal distribution with a mean of 0 and a standard deviation of 1.

They showed that with this activation function and this initialization scheme, the variance of the outputs of each layer is much greater than the variance of its inputs. Going forward in the network, the variance keeps increasing after each layer until the activation function saturates at the top layers. This is actually made worse by the fact that the logistic function has a mean of 0.5, not 0 (the hyperbolic tangent function has a mean of 0 and behaves slightly better than the logistic function in deep networks).

The derivative of the Logistic funtion

Looking at the logistic activation function, when inputs become large (negative or positive), the function saturates at 0 or 1, with a derivative extremely close to 0. Thus when backpropagation kicks in, it has virtually no gradient to propagate back through the network, and what little gradient exists keeps getting diluted as backpropagation progresses down through the top layers, so there is really nothing left for the lower layers.

In their paper, Glorot and Bengio propose a way to significantly alleviate this problem. We need the signal to flow properly in both directions: in the forward direction when making predictions, and in the reverse direction when backpropagating gradients. We don't want the signal to die out, nor do we want it to explode and saturate. For the signal to flow properly, the authors argue that we need the variance of the outputs of each layer to be equal to the variance of its inputs, and we also need the gradients to have equal variance before and after flowing through a layer in the reverse direction.

Insights from the paper by Glorot and Bengio

One of the insights in the 2010 paper by Glorot and Bengio was that the vanishing/exploding gradients problems were in part due to a poor choice of activation function. Until then most people had assumed that if Nature had chosen to use roughly sigmoid activation functions in biological neurons, they must be an excellent choice. But it turns out that other activation functions behave much better in deep neural networks, in particular the ReLU activation function, mostly because it does not saturate for positive values (and also because it is quite fast to compute).

The RELU function family

The ReLU activation function suffers from a problem known as the dying ReLUs: during training, some neurons effectively die, meaning they stop outputting anything other than 0.

In some cases, you may find that half of your network's neurons are dead, especially if you used a large learning rate. During training, if a neuron's weights get updated such that the weighted sum of the neuron's inputs is negative, it will start outputting 0. When this happen, the neuron is unlikely to come back to life since the gradient of the ReLU function is 0 when its input is negative.

To solve this problem, nowadays practitioners use a variant of the ReLU function, such as the leaky ReLU discussed above or the so-called exponential linear unit (ELU) function

$$ELU(z) = \left\{ \begin{array}{cc} \alpha\left(\exp\left(z\right) - 1\right) & z < 0, \\ z & z \geq 0. \end{array} \right.$$

Which activation function should we use?

In general it seems that the ELU activation function is better than the leaky ReLU function (and its variants), which is better than ReLU. ReLU performs better than tanh which in turn performs better than the logistic function.

If runtime performance is an issue, then you may opt for the leaky ReLU function over the ELU function If you don't want to tweak yet another hyperparameter, you may just use the default α of 0.01 for the leaky ReLU, and 1 for ELU. If you have spare time and computing power, you can use cross-validation or bootstrap to evaluate other activation functions.

More on activation functions, output layers

In most cases you can use the ReLU activation function in the hidden layers (or one of its variants).

It is a bit faster to compute than other activation functions, and the gradient descent optimization does in general not get stuck.

For the output layer:

- For classification the softmax activation function is generally a good choice for classification tasks (when the classes are mutually exclusive).
- For regression tasks, you can simply use no activation function at all.

Batch Normalization

Batch Normalization aims to address the vanishing/exploding gradients problems, and more generally the problem that the distribution of each layer's inputs changes during training, as the parameters of the previous layers change.

The technique consists of adding an operation in the model just before the activation function of each layer, simply zero-centering and normalizing the inputs, then scaling and shifting the result using two new parameters per layer (one for scaling, the other for shifting). In other words, this operation lets the model learn the optimal scale and mean of the inputs for each layer. In order to zero-center and normalize the inputs, the algorithm needs to estimate the inputs' mean and standard deviation. It does so by evaluating the mean and standard deviation of the inputs over the current mini-batch, from this the name batch normalization.

Dropout

It is a fairly simple algorithm: at every training step, every neuron (including the input neurons but excluding the output neurons) has a probability p of being temporarily dropped out, meaning it will be entirely ignored during this training step, but it may be active during the next step.

The hyperparameter p is called the dropout rate, and it is typically set to 50%. After training, the neurons are not dropped anymore. It is viewed as one of the most popular regularization techniques.

Gradient Clipping

A popular technique to lessen the exploding gradients problem is to simply clip the gradients during backpropagation so that they never exceed some threshold (this is mostly useful for recurrent neural networks).

This technique is called Gradient Clipping.

In general however, Batch Normalization is preferred.

A top-down perspective on Neural networks

The first thing we would like to do is divide the data into two or three parts. A training set, a validation or dev (development) set, and a test set. The test set is the data on which we want to make predictions. The dev set is a subset of the training data we use to check how well we are doing out-of-sample, after training the model on the training dataset. We use the validation error as a proxy for the test error in order to make tweaks to our model. It is crucial that we do not use any of the test data to train the algorithm. This is a cardinal sin in ML. Then:

- Estimate optimal error rate
- Minimize underfitting (bias) on training data set.
- Make sure you are not overfitting.

More top-down perspectives

If the validation and test sets are drawn from the same distributions, then a good performance on the validation set should lead to similarly good performance on the test set.

However, sometimes the training data and test data differ in subtle ways because, for example, they are collected using slightly different methods, or because it is cheaper to collect data in one way versus another. In this case, there can be a mismatch between the training and test data. This can lead to the neural network overfitting these small differences between the test and training sets, and a poor performance on the test set despite having a good performance on the validation set. To rectify this, Andrew Ng suggests making two validation or dev sets, one constructed from the training data and one constructed from the test data. The difference between the performance of the algorithm on these two validation sets quantifies the train-test mismatch. This can serve as another important diagnostic when using DNNs for supervised learning.

Limitations of supervised learning with deep networks

Like all statistical methods, supervised learning using neural networks has important limitations. This is especially important when one seeks to apply these methods, especially to physics problems. Like all tools, DNNs are not a universal solution. Often, the same or better performance on a task can be achieved by using a few hand-engineered features (or even a collection of random features).

Limitations of NNs

Here we list some of the important limitations of supervised neural network based models.

- **Need labeled data**. All supervised learning methods, DNNs for supervised learning require labeled data. Often, labeled data is harder to acquire than unlabeled data (e.g. one must pay for human experts to label images).
- **Supervised neural networks are extremely data intensive.** DNNs are data hungry. They perform best when data is plentiful. This is doubly so for supervised methods where the data must also be labeled. The utility of DNNs is extremely limited if data is hard to acquire or the datasets are small (hundreds to a few thousand samples). In this case, the performance of other methods that utilize hand-engineered features can exceed that of DNNs.

Homogeneous data

- **Homogeneous data.** Almost all DNNs deal with homogeneous data of one type. It is very hard to design architectures that mix and match data types (i.e. some continuous variables, some discrete variables, some time series). In applications beyond images, video, and language, this is often what is required. In contrast, ensemble models like random forests or gradient-boosted trees have no difficulty handling mixed data types.

More limitations

- **Many problems are not about prediction.** In natural science we are often interested in learning something about the underlying distribution that generates the data. In this case, it is often difficult to cast these ideas in a supervised learning setting. While the problems are related, it is possible to make good predictions with a *wrong* model. The model might or might not be useful for understanding the underlying science.

Some of these remarks are particular to DNNs, others are shared by all supervised learning methods. This motivates the use of unsupervised methods which in part circumvent these problems.

Building a neural network code

Here we present a flexible object oriented codebase for a feed forward neural network, along with a demonstration of how to use it. Before we get into the details of the neural network, we will first present some implementations of various schedulers, cost functions and activation functions that can be used together with the neural network.

The codes here were developed by Eric Reber and Gregor Kajda during spring 2023. After these codes we present the TensorFlow inplementation. Pytorch will be discussed next week.

Learning rate methods

The code below shows object oriented implementations of the Constant, Momentum, Adagrad, AdagradMomentum, RMS prop and Adam schedulers. All of the classes belong to the shared abstract **Scheduler class**, and share the update_change() and reset() methods allowing for any of the schedulers to be seamlessly used during the training stage, as will later be shown in the fit() method of the neural network. Update_change() only has one parameter, the gradient, and returns the change which will be subtracted from the weights. The reset() function takes no parameters, and resets the desired variables. For Constant and Momentum, reset does nothing.

```
import autograd.numpy as np

class Scheduler:
    """
    Abstract class for Schedulers
    """

    def __init__(self, eta):
        self.eta = eta

    # should be overwritten
    def update_change(self, gradient):
        raise NotImplementedError

    # overwritten if needed
    def reset(self):
        pass


class Constant(Scheduler):
    def __init__(self, eta):
        super().__init__(eta)
```

```python
    def update_change(self, gradient):
        return self.eta * gradient

    def reset(self):
        pass


class Momentum(Scheduler):
    def __init__(self, eta: float, momentum: float):
        super().__init__(eta)
        self.momentum = momentum
        self.change = 0

    def update_change(self, gradient):
        self.change = self.momentum * self.change + self.eta * gradient
        return self.change

    def reset(self):
        pass


class Adagrad(Scheduler):
    def __init__(self, eta):
        super().__init__(eta)
        self.G_t = None

    def update_change(self, gradient):
        delta = 1e-8  # avoid division ny zero

        if self.G_t is None:
            self.G_t = np.zeros((gradient.shape[0], gradient.shape[0]))

        self.G_t += gradient @ gradient.T

        G_t_inverse = 1 / (
            delta + np.sqrt(np.reshape(np.diagonal(self.G_t), (self.G_t.shape[0], 1)))
        )
        return self.eta * gradient * G_t_inverse

    def reset(self):
        self.G_t = None


class AdagradMomentum(Scheduler):
    def __init__(self, eta, momentum):
        super().__init__(eta)
        self.G_t = None
        self.momentum = momentum
        self.change = 0

    def update_change(self, gradient):
        delta = 1e-8  # avoid division ny zero

        if self.G_t is None:
            self.G_t = np.zeros((gradient.shape[0], gradient.shape[0]))

        self.G_t += gradient @ gradient.T

        G_t_inverse = 1 / (
            delta + np.sqrt(np.reshape(np.diagonal(self.G_t), (self.G_t.shape[0], 1)))
        )
        self.change = self.change * self.momentum + self.eta * gradient * G_t_inverse
        return self.change

    def reset(self):
        self.G_t = None


class RMS_prop(Scheduler):
    def __init__(self, eta, rho):
        super().__init__(eta)
        self.rho = rho
        self.second = 0.0

    def update_change(self, gradient):
        delta = 1e-8  # avoid division ny zero
        self.second = self.rho * self.second + (1 - self.rho) * gradient * gradient
        return self.eta * gradient / (np.sqrt(self.second + delta))

    def reset(self):
        self.second = 0.0


class Adam(Scheduler):
    def __init__(self, eta, rho, rho2):
        super().__init__(eta)
        self.rho = rho
        self.rho2 = rho2
        self.moment = 0
        self.second = 0
        self.n_epochs = 1

    def update_change(self, gradient):
        delta = 1e-8  # avoid division ny zero

        self.moment = self.rho * self.moment + (1 - self.rho) * gradient
        self.second = self.rho2 * self.second + (1 - self.rho2) * gradient * gradient

        moment_corrected = self.moment / (1 - self.rho**self.n_epochs)
        second_corrected = self.second / (1 - self.rho2**self.n_epochs)

        return self.eta * moment_corrected / (np.sqrt(second_corrected + delta))

    def reset(self):
        self.n_epochs += 1
        self.moment = 0
        self.second = 0
```

Usage of the above learning rate schedulers

To initalize a scheduler, simply create the object and pass in the necessary parameters such as the learning rate and the momentum as shown below. As the Scheduler class is an abstract class it should not called directly, and will raise an error upon usage.

```
momentum_scheduler = Momentum(eta=1e-3, momentum=0.9)
adam_scheduler = Adam(eta=1e-3, rho=0.9, rho2=0.999)
```

Here is a small example for how a segment of code using schedulers could look. Switching out the schedulers is simple.

```
weights = np.ones((3,3))
print(f"Before scheduler:\n{weights=}")

epochs = 10
for e in range(epochs):
    gradient = np.random.rand(3, 3)
    change = adam_scheduler.update_change(gradient)
    weights = weights - change
    adam_scheduler.reset()

print(f"\nAfter scheduler:\n{weights=}")
```

Cost functions

Here we discuss cost functions that can be used when creating the neural network. Every cost function takes the target vector as its parameter, and returns a function valued only at x such that it may easily be differentiated.

```
import autograd.numpy as np

def CostOLS(target):

    def func(X):
        return (1.0 / target.shape[0]) * np.sum((target - X) ** 2)

    return func


def CostLogReg(target):

    def func(X):

        return -(1.0 / target.shape[0]) * np.sum(
            (target * np.log(X + 10e-10)) + ((1 - target) * np.log(1 - X + 10e-10))
        )

    return func


def CostCrossEntropy(target):

    def func(X):
        return -(1.0 / target.size) * np.sum(target * np.log(X + 10e-10))

    return func
```

Below we give a short example of how these cost function may be used to obtain results if you wish to test them out on your own using AutoGrad's automatics differentiation.

```
from autograd import grad

target = np.array([[1, 2, 3]]).T
a = np.array([[4, 5, 6]]).T

cost_func = CostCrossEntropy
cost_func_derivative = grad(cost_func(target))

valued_at_a = cost_func_derivative(a)
print(f"Derivative of cost function {cost_func.__name__} valued at a:\n{valued_at_a}")
```

Activation functions

Finally, before we look at the neural network, we will look at the activation functions which can be specified between the hidden layers and as the output function. Each function can be valued for any given vector or matrix X, and can be differentiated via derivate().

```
import autograd.numpy as np
from autograd import elementwise_grad

def identity(X):
    return X


def sigmoid(X):
    try:
        return 1.0 / (1 + np.exp(-X))
    except FloatingPointError:
        return np.where(X > np.zeros(X.shape), np.ones(X.shape), np.zeros(X.shape))


def softmax(X):
    X = X - np.max(X, axis=-1, keepdims=True)
    delta = 10e-10
    return np.exp(X) / (np.sum(np.exp(X), axis=-1, keepdims=True) + delta)


def RELU(X):
    return np.where(X > np.zeros(X.shape), X, np.zeros(X.shape))


def LRELU(X):
    delta = 10e-4
    return np.where(X > np.zeros(X.shape), X, delta * X)


def derivate(func):
    if func.__name__ == "RELU":

        def func(X):
            return np.where(X > 0, 1, 0)

        return func

    elif func.__name__ == "LRELU":

        def func(X):
            delta = 10e-4
            return np.where(X > 0, 1, delta)

        return func

    else:
        return elementwise_grad(func)
```

Below follows a short demonstration of how to use an activation function. The derivative of the activation function will be important when calculating the output delta term during backpropagation. Note that derivate() can also be used for cost functions for a more generalized approach.

```
z = np.array([[4, 5, 6]]).T
print(f"Input to activation function:\n{z}")

act_func = sigmoid
a = act_func(z)
print(f"\nOutput from {act_func.__name__} activation function:\n{a}")

act_func_derivative = derivate(act_func)
valued_at_z = act_func_derivative(a)
print(f"\nDerivative of {act_func.__name__} activation function valued at z:\n{valued_at_z}")
```

The Neural Network

Now that we have gotten a good understanding of the implementation of some important components, we can take a look at an object oriented implementation of a feed forward neural network. The feed forward neural network has been implemented as a class named FFNN, which can be initiated as a regressor or classifier dependant on the choice of cost function. The FFNN can have any number of input nodes, hidden layers with any amount of hidden nodes, and any amount of output nodes meaning it can perform multiclass classification as well as binary classification and regression problems. Although there is a lot of code present, it makes for an easy to use and generalizeable interface for creating many types of neural networks as will be demonstrated below.

```
import math
import autograd.numpy as np
import sys
import warnings
from autograd import grad, elementwise_grad
from random import random, seed
from copy import deepcopy, copy
from typing import Tuple, Callable
from sklearn.utils import resample

warnings.simplefilter("error")


class FFNN:
    """
    Description:
```

```
------------
    Feed Forward Neural Network with interface enabling flexible design of a
    nerual networks architecture and the specification of activation function
    in the hidden layers and output layer respectively. This model can be used
    for both regression and classification problems, depending on the output function.

Attributes:
------------
    I   dimensions (tuple[int]): A list of positive integers, which specifies the
        number of nodes in each of the networks layers. The first integer in the array
        defines the number of nodes in the input layer, the second integer defines number
        of nodes in the first hidden layer and so on until the last number, which
        specifies the number of nodes in the output layer.
    II  hidden_func (Callable): The activation function for the hidden layers
    III output_func (Callable): The activation function for the output layer
    IV  cost_func (Callable): Our cost function
    V   seed (int): Sets random seed, makes results reproducible
"""

def __init__(
    self,
    dimensions: tuple[int],
    hidden_func: Callable = sigmoid,
    output_func: Callable = lambda x: x,
    cost_func: Callable = CostOLS,
    seed: int = None,
):
    self.dimensions = dimensions
    self.hidden_func = hidden_func
    self.output_func = output_func
    self.cost_func = cost_func
    self.seed = seed
    self.weights = list()
    self.schedulers_weight = list()
    self.schedulers_bias = list()
    self.a_matrices = list()
    self.z_matrices = list()
    self.classification = None

    self.reset_weights()
    self._set_classification()

def fit(
    self,
    X: np.ndarray,
    t: np.ndarray,
    scheduler: Scheduler,
    batches: int = 1,
    epochs: int = 100,
    lam: float = 0,
    X_val: np.ndarray = None,
    t_val: np.ndarray = None,
):
    """
    Description:
    ------------
        This function performs the training the neural network by performing the feedforward
        algorithm to update the networks weights.

    Parameters:
    ------------
    I    X (np.ndarray) : training data
    II   t (np.ndarray) : target data
    III  scheduler (Scheduler) : specified scheduler (algorithm for optimization of gradi
    IV   scheduler_args (list[int]) : list of all arguments necessary for scheduler

Optional Parameters:
------------
    V    batches (int) : number of batches the datasets are split into, default equal to
    VI   epochs (int) : number of iterations used to train the network, default equal to
    VII  lam (float) : regularization hyperparameter lambda
    VIII X_val (np.ndarray) : validation set
    IX   t_val (np.ndarray) : validation target set

Returns:
------------
    I   scores (dict) : A dictionary containing the performance metrics of the model.
        The number of the metrics depends on the parameters passed to the fit-function.

"""

# setup
if self.seed is not None:
    np.random.seed(self.seed)

val_set = False
if X_val is not None and t_val is not None:
    val_set = True

# creating arrays for score metrics
train_errors = np.empty(epochs)
train_errors.fill(np.nan)
val_errors = np.empty(epochs)
val_errors.fill(np.nan)

train_accs = np.empty(epochs)
train_accs.fill(np.nan)
val_accs = np.empty(epochs)
val_accs.fill(np.nan)

self.schedulers_weight = list()
self.schedulers_bias = list()

batch_size = X.shape[0] // batches

X, t = resample(X, t)

# this function returns a function valued only at X
cost_function_train = self.cost_func(t)
if val_set:
    cost_function_val = self.cost_func(t_val)

# create schedulers for each weight matrix
for i in range(len(self.weights)):
    self.schedulers_weight.append(copy(scheduler))
    self.schedulers_bias.append(copy(scheduler))

print(f"{scheduler.__class__.__name__}: Eta={scheduler.eta}, Lambda={lam}")

try:
    for e in range(epochs):
        for i in range(batches):
            # allows for minibatch gradient descent
            if i == batches - 1:
                # If the for loop has reached the last batch, take all thats left
                X_batch = X[i * batch_size :, :]
                t_batch = t[i * batch_size :, :]
            else:
                X_batch = X[i * batch_size : (i + 1) * batch_size, :]
                t_batch = t[i * batch_size : (i + 1) * batch_size, :]

            self._feedforward(X_batch)
            self._backpropagate(X_batch, t_batch, lam)

        # reset schedulers for each epoch (some schedulers pass in this call)
        for scheduler in self.schedulers_weight:
            scheduler.reset()

        for scheduler in self.schedulers_bias:
            scheduler.reset()

        # computing performance metrics
        pred_train = self.predict(X)
        train_error = cost_function_train(pred_train)

        train_errors[e] = train_error
        if val_set:

            pred_val = self.predict(X_val)
            val_error = cost_function_val(pred_val)
            val_errors[e] = val_error

        if self.classification:
            train_acc = self._accuracy(self.predict(X), t)
            train_accs[e] = train_acc
            if val_set:
                val_acc = self._accuracy(pred_val, t_val)
                val_accs[e] = val_acc

        # printing progress bar
        progression = e / epochs
        print_length = self._progress_bar(
            progression,
            train_error=train_errors[e],
            train_acc=train_accs[e],
            val_error=val_errors[e],
            val_acc=val_accs[e],
        )
except KeyboardInterrupt:
    # allows for stopping training at any point and seeing the result
    pass

# visualization of training progression (similiar to tensorflow progression bar)
sys.stdout.write("\r" + " " * print_length)
sys.stdout.flush()
self._progress_bar(
    1,
    train_error=train_errors[e],
    train_acc=train_accs[e],
    val_error=val_errors[e],
    val_acc=val_accs[e],
)
sys.stdout.write("")
```

```
        # return performance metrics for the entire run
        scores = dict()

        scores["train_errors"] = train_errors

        if val_set:
            scores["val_errors"] = val_errors

        if self.classification:
            scores["train_accs"] = train_accs

            if val_set:
                scores["val_accs"] = val_accs

        return scores

    def predict(self, X: np.ndarray, *, threshold=0.5):
        """
         Description:
         ------------
             Performs prediction after training of the network has been finished.

         Parameters:
        ------------
             I   X (np.ndarray): The design matrix, with n rows of p features each

         Optional Parameters:
         ------------
             II  threshold (float) : sets minimal value for a prediction to be predicted as the p
                 in classification problems

         Returns:
         ------------
             I   z (np.ndarray): A prediction vector (row) for each row in our design matrix
                 This vector is thresholded if regression=False, meaning that classification resu
                 in a vector of 1s and 0s, while regressions in an array of decimal numbers

        """

        predict = self._feedforward(X)

        if self.classification:
            return np.where(predict > threshold, 1, 0)
        else:
            return predict

    def reset_weights(self):
        """
        Description:
        ------------
            Resets/Reinitializes the weights in order to train the network for a new problem.

        """
        if self.seed is not None:
            np.random.seed(self.seed)

        self.weights = list()
        for i in range(len(self.dimensions) - 1):
            weight_array = np.random.randn(
                self.dimensions[i] + 1, self.dimensions[i + 1]
            )
            weight_array[0, :] = np.random.randn(self.dimensions[i + 1]) * 0.01

            self.weights.append(weight_array)

    def _feedforward(self, X: np.ndarray):
        """
        Description:
        ------------
            Calculates the activation of each layer starting at the input and ending at the outpu
            Each following activation is calculated from a weighted sum of each of the preceeding
            activations (except in the case of the input layer).

        Parameters:
        ------------
            I   X (np.ndarray): The design matrix, with n rows of p features each

        Returns:
        ------------
            I   z (np.ndarray): A prediction vector (row) for each row in our design matrix
        """

        # reset matrices
        self.a_matrices = list()
        self.z_matrices = list()

        # if X is just a vector, make it into a matrix
        if len(X.shape) == 1:
            X = X.reshape((1, X.shape[0]))

        # Add a coloumn of zeros as the first coloumn of the design matrix, in order
        # to add bias to our data
        bias = np.ones((X.shape[0], 1)) * 0.01
        X = np.hstack([bias, X])

        # a^0, the nodes in the input layer (one a^0 for each row in X - where the
        # exponent indicates layer number).
        a = X
        self.a_matrices.append(a)
        self.z_matrices.append(a)

        # The feed forward algorithm
        for i in range(len(self.weights)):
            if i < len(self.weights) - 1:
                z = a @ self.weights[i]
                self.z_matrices.append(z)
                a = self.hidden_func(z)
                # bias column again added to the data here
                bias = np.ones((a.shape[0], 1)) * 0.01
                a = np.hstack([bias, a])
                self.a_matrices.append(a)
            else:
                try:
                    # a^L, the nodes in our output layers
                    z = a @ self.weights[i]
                    a = self.output_func(z)
                    self.a_matrices.append(a)
                    self.z_matrices.append(z)
                except Exception as OverflowError:
                    print(
                        "OverflowError in fit() in FFNN\nHOW TO DEBUG ERROR: Consider lowering you
            )

        # this will be a^L
        return a

    def _backpropagate(self, X, t, lam):
        """
        Description:
        ------------
            Performs the backpropagation algorithm. In other words, this method
            calculates the gradient of all the layers starting at the
            output layer, and moving from right to left accumulates the gradient until
            the input layer is reached. Each layers respective weights are updated while
            the algorithm propagates backwards from the output layer (auto-differentation in reve

        Parameters:
        ------------
            I   X (np.ndarray): The design matrix, with n rows of p features each.
            II  t (np.ndarray): The target vector, with n rows of p targets.
            III lam (float32): regularization parameter used to punish the weights in case of ove

        Returns:
        ------------
            No return value.

        """
        out_derivative = derivate(self.output_func)
        hidden_derivative = derivate(self.hidden_func)

        for i in range(len(self.weights) - 1, -1, -1):
            # delta terms for output
            if i == len(self.weights) - 1:
                # for multi-class classification
                if (
                    self.output_func.__name__ == "softmax"
                ):
                    delta_matrix = self.a_matrices[i + 1] - t
                # for single class classification
                else:
                    cost_func_derivative = grad(self.cost_func(t))
                    delta_matrix = out_derivative(
                        self.z_matrices[i + 1]
                    ) * cost_func_derivative(self.a_matrices[i + 1])

            # delta terms for hidden layer
            else:
                delta_matrix = (
                    self.weights[i + 1][1:, :] @ delta_matrix.T
                ).T * hidden_derivative(self.z_matrices[i + 1])

            # calculate gradient
            gradient_weights = self.a_matrices[i][:, 1:].T @ delta_matrix
            gradient_bias = np.sum(delta_matrix, axis=0).reshape(
                1, delta_matrix.shape[1]
            )

            # regularization term
            gradient_weights += self.weights[i][1:, :] * lam

            # use scheduler
            update_matrix = np.vstack(
                [
                    self.schedulers_bias[i].update_change(gradient_bias),
                    self.schedulers_weight[i].update_change(gradient_weights),
                ]
            )

            # update weights and bias
            self.weights[i] -= update_matrix

    def _accuracy(self, prediction: np.ndarray, target: np.ndarray):
        """
        Description:
        ------------
            Calculates accuracy of given prediction to target

        Parameters:
        ------------
            I   prediction (np.ndarray): vector of predicitons output network
                (1s and 0s in case of classification, and real numbers in case of regression)
            II  target (np.ndarray): vector of true values (What the network ideally should predi

        Returns:
        ------------
            A floating point number representing the percentage of correctly classified instances
        """
        assert prediction.size == target.size
        return np.average((target == prediction))
    def _set_classification(self):
        """
        Description:
        ------------
            Decides if FFNN acts as classifier (True) og regressor (False),
            sets self.classification during init()
        """
        self.classification = False
        if (
            self.cost_func.__name__ == "CostLogReg"
            or self.cost_func.__name__ == "CostCrossEntropy"
        ):
            self.classification = True

    def _progress_bar(self, progression, **kwargs):
        """
        Description:
        ------------
            Displays progress of training
        """
        print_length = 40
        num_equals = int(progression * print_length)
        num_not = print_length - num_equals
        arrow = ">" if num_equals > 0 else ""
        bar = "[" + "=" * (num_equals - 1) + arrow + "-" * num_not + "]"
        perc_print = self._format(progression * 100, decimals=5)
        line = f"  {bar} {perc_print}% "

        for key in kwargs:
            if not np.isnan(kwargs[key]):
                value = self._format(kwargs[key], decimals=4)
                line += f"| {key}: {value} "
        sys.stdout.write("\r" + line)
        sys.stdout.flush()
```

```
            return len(line)

        def _format(self, value, decimals=4):
            """
            Description:
            ------------
                Formats decimal numbers for progress bar
            """
            if value > 0:
                v = value
            elif value < 0:
                v = -10 * value
            else:
                v = 1
            n = 1 + math.floor(math.log10(v))
            if n >= decimals - 1:
                return str(round(value))
            return f"{value:.{decimals-n-1}f}"
```

Before we make a model, we will quickly generate a dataset we can use for our linear regression problem as shown below

```
import autograd.numpy as np
from sklearn.model_selection import train_test_split

def SkrankeFunction(x, y):
    return np.ravel(0 + 1*x + 2*y + 3*x**2 + 4*x*y + 5*y**2)

def create_X(x, y, n):
    if len(x.shape) > 1:
        x = np.ravel(x)
        y = np.ravel(y)

    N = len(x)
    l = int((n + 1) * (n + 2) / 2)  # Number of elements in beta
    X = np.ones((N, l))

    for i in range(1, n + 1):
        q = int((i) * (i + 1) / 2)
        for k in range(i + 1):
            X[:, q + k] = (x ** (i - k)) * (y**k)

    return X

step=0.5
x = np.arange(0, 1, step)
y = np.arange(0, 1, step)
x, y = np.meshgrid(x, y)
target = SkrankeFunction(x, y)
target = target.reshape(target.shape[0], 1)

poly_degree=3
X = create_X(x, y, poly_degree)

X_train, X_test, t_train, t_test = train_test_split(X, target)
```

Now that we have our dataset ready for the regression, we can create our regressor. Note that with the seed parameter, we can make sure our results stay the same every time we run the neural network. For inititialization, we simply specify the dimensions (we wish the amount of input nodes to be equal to the datapoints, and the output to predict one value).

```
input_nodes = X_train.shape[1]
output_nodes = 1

linear_regression = FFNN((input_nodes, output_nodes), output_func=identity, cost_func=CostOLS, see
```

We then fit our model with our training data using the scheduler of our choice.

```
linear_regression.reset_weights() # reset weights such that previous runs or reruns don't affect

scheduler = Constant(eta=1e-3)
scores = linear_regression.fit(X_train, t_train, scheduler)
```

Due to the progress bar we can see the MSE (train_error) throughout the FFNN's training. Note that the fit() function has some optional parameters with defualt arguments. For example, the regularization hyperparameter can be left ignored if not needed, and equally the FFNN will by default run for 100 epochs. These can easily be changed, such as for example:

```
linear_regression.reset_weights() # reset weights such that previous runs or reruns don't affect

scores = linear_regression.fit(X_train, t_train, scheduler, lam=1e-4, epochs=1000)
```

We see that given more epochs to train on, the regressor reaches a lower MSE.

Let us then switch to a binary classification. We use a binary classification dataset, and follow a similar setup to the regression case.

```
from sklearn.datasets import load_breast_cancer
from sklearn.preprocessing import MinMaxScaler

wisconsin = load_breast_cancer()
X = wisconsin.data
target = wisconsin.target
target = target.reshape(target.shape[0], 1)

X_train, X_val, t_train, t_val = train_test_split(X, target)

scaler = MinMaxScaler()
scaler.fit(X_train)
X_train = scaler.transform(X_train)
X_val = scaler.transform(X_val)
```

```
input_nodes = X_train.shape[1]
output_nodes = 1

logistic_regression = FFNN((input_nodes, output_nodes), output_func=sigmoid, cost_func=CostLogReg
```

We will now make use of our validation data by passing it into our fit function as a keyword argument

```
logistic_regression.reset_weights() # reset weights such that previous runs or reruns don't affec

scheduler = Adam(eta=1e-3, rho=0.9, rho2=0.999)
scores = logistic_regression.fit(X_train, t_train, scheduler, epochs=1000, X_val=X_val, t_val=t_va
```

Finally, we will create a neural network with 2 hidden layers with activation functions.

```
input_nodes = X_train.shape[1]
hidden_nodes1 = 100
hidden_nodes2 = 30
output_nodes = 1

dims = (input_nodes, hidden_nodes1, hidden_nodes2, output_nodes)

neural_network = FFNN(dims, hidden_func=RELU, output_func=sigmoid, cost_func=CostLogReg, seed=2023
```

```
neural_network.reset_weights() # reset weights such that previous runs or reruns don't affect the

scheduler = Adam(eta=1e-4, rho=0.9, rho2=0.999)
scores = neural_network.fit(X_train, t_train, scheduler, epochs=1000, X_val=X_val, t_val=t_val)
```

Multiclass classification

Finally, we will demonstrate the use case of multiclass classification using our FFNN with the famous MNIST dataset, which contain images of digits between the range of 0 to 9.

```
from sklearn.datasets import load_digits

def onehot(target: np.ndarray):
    onehot = np.zeros((target.size, target.max() + 1))
    onehot[np.arange(target.size), target] = 1
    return onehot

digits = load_digits()

X = digits.data
target = digits.target
target = onehot(target)

input_nodes = 64
hidden_nodes1 = 100
hidden_nodes2 = 30
output_nodes = 10

dims = (input_nodes, hidden_nodes1, hidden_nodes2, output_nodes)

multiclass = FFNN(dims, hidden_func=LRELU, output_func=softmax, cost_func=CostCrossEntropy)

multiclass.reset_weights() # reset weights such that previous runs or reruns don't affect the wei

scheduler = Adam(eta=1e-4, rho=0.9, rho2=0.999)
scores = multiclass.fit(X, target, scheduler, epochs=1000)
```

Testing the XOR gate and other gates

Let us now use our code to test the XOR gate.

```
X = np.array([ [0, 0], [0, 1], [1, 0],[1, 1]],dtype=np.float64)

# The XOR gate
yXOR = np.array( [[ 0], [1] ,[1], [0]])

input_nodes = X.shape[1]
output_nodes = 1

logistic_regression = FFNN((input_nodes, output_nodes), output_func=sigmoid, cost_func=CostLogReg
logistic_regression.reset_weights() # reset weights such that previous runs or reruns don't affec
scheduler = Adam(eta=1e-1, rho=0.9, rho2=0.999)
scores = logistic_regression.fit(X, yXOR, scheduler, epochs=1000)
```

Not bad, but the results depend strongly on the learning reate. Try different learning rates.

Building neural networks in Tensorflow and Keras

Now we want to build on the experience gained from our neural network implementation in NumPy and scikit-learn and use it to construct a neural network in Tensorflow. Once we have constructed a neural network in NumPy and Tensorflow, building one in Keras is really quite trivial, though the performance may suffer.

In our previous example we used only one hidden layer, and in this we will use two. From this it should be quite clear how to build one using an arbitrary number of hidden layers, using data structures such as Python lists or NumPy arrays.

Tensorflow

Tensorflow is an open source library machine learning library developed by the Google Brain team for internal use. It was released under the Apache 2.0 open source license in November 9, 2015.

Tensorflow is a computational framework that allows you to construct machine learning models at different levels of abstraction, from high-level, object-oriented APIs like Keras, down to the C++ kernels that Tensorflow is built upon. The higher levels of abstraction are simpler to use, but less flexible, and our choice of implementation should reflect the problems we are trying to solve.

Tensorflow uses so-called graphs to represent your computation in terms of the dependencies between individual operations, such that you first build a Tensorflow *graph* to represent your model, and then create a Tensorflow *session* to run the graph.

In this guide we will analyze the same data as we did in our NumPy and scikit-learn tutorial, gathered from the MNIST database of images. We will give an introduction to the lower level Python Application Program Interfaces (APIs), and see how we use them to build our graph. Then we will build (effectively) the same graph in Keras, to see just how simple solving a machine learning problem can be.

To install tensorflow on Unix/Linux systems, use pip as

```
pip3 install tensorflow
```

and/or if you use **anaconda**, just write (or install from the graphical user interface) (current release of CPU-only TensorFlow)

```
conda create -n tf tensorflow
conda activate tf
```

To install the current release of GPU TensorFlow

```
conda create -n tf-gpu tensorflow-gpu
conda activate tf-gpu
```

Using Keras

Keras is a high level neural network that supports Tensorflow, CTNK and Theano as backends. If you have Anaconda installed you may run the following command

```
conda install keras
```

You can look up the instructions here for more information.

We will to a large extent use **keras** in this course.

Collect and pre-process data

Let us look again at the MINST data set.

```
# import necessary packages
import numpy as np
import matplotlib.pyplot as plt
import tensorflow as tf
from sklearn import datasets


# ensure the same random numbers appear every time
np.random.seed(0)

# display images in notebook
%matplotlib inline
plt.rcParams['figure.figsize'] = (12,12)


# download MNIST dataset
digits = datasets.load_digits()

# define inputs and labels
inputs = digits.images
labels = digits.target

print("inputs = (n_inputs, pixel_width, pixel_height) = " + str(inputs.shape))
print("labels = (n_inputs) = " + str(labels.shape))


# flatten the image
# the value -1 means dimension is inferred from the remaining dimensions: 8x8 = 64
n_inputs = len(inputs)
inputs = inputs.reshape(n_inputs, -1)
print("X = (n_inputs, n_features) = " + str(inputs.shape))


# choose some random images to display
indices = np.arange(n_inputs)
random_indices = np.random.choice(indices, size=5)

for i, image in enumerate(digits.images[random_indices]):
    plt.subplot(1, 5, i+1)
    plt.axis('off')
    plt.imshow(image, cmap=plt.cm.gray_r, interpolation='nearest')
    plt.title("Label: %d" % digits.target[random_indices[i]])
plt.show()


from tensorflow.keras.layers import Input
from tensorflow.keras.models import Sequential      #This allows appending layers to existing mode
from tensorflow.keras.layers import Dense           #This allows defining the characteristics of
from tensorflow.keras import optimizers             #This allows using whichever optimiser we wan
from tensorflow.keras import regularizers           #This allows using whichever regularizer we w
from tensorflow.keras.utils import to_categorical   #This allows using categorical cross entropy

from sklearn.model_selection import train_test_split

# one-hot representation of labels
labels = to_categorical(labels)
```

```python
# split into train and test data
train_size = 0.8
test_size = 1 - train_size
X_train, X_test, Y_train, Y_test = train_test_split(inputs, labels, train_size=train_size,
                                                    test_size=test_size)



epochs = 100
batch_size = 100
n_neurons_layer1 = 100
n_neurons_layer2 = 50
n_categories = 10
eta_vals = np.logspace(-5, 1, 7)
lmbd_vals = np.logspace(-5, 1, 7)
def create_neural_network_keras(n_neurons_layer1, n_neurons_layer2, n_categories, eta, lmbd):
    model = Sequential()
    model.add(Dense(n_neurons_layer1, activation='sigmoid', kernel_regularizer=regularizers.l2(lmb
    model.add(Dense(n_neurons_layer2, activation='sigmoid', kernel_regularizer=regularizers.l2(lmb
    model.add(Dense(n_categories, activation='softmax'))

    sgd = optimizers.SGD(lr=eta)
    model.compile(loss='categorical_crossentropy', optimizer=sgd, metrics=['accuracy'])

    return model


DNN_keras = np.zeros((len(eta_vals), len(lmbd_vals)), dtype=object)

for i, eta in enumerate(eta_vals):
    for j, lmbd in enumerate(lmbd_vals):
        DNN = create_neural_network_keras(n_neurons_layer1, n_neurons_layer2, n_categories,
                                          eta=eta, lmbd=lmbd)
        DNN.fit(X_train, Y_train, epochs=epochs, batch_size=batch_size, verbose=0)
        scores = DNN.evaluate(X_test, Y_test)

        DNN_keras[i][j] = DNN

        print("Learning rate = ", eta)
        print("Lambda = ", lmbd)
        print("Test accuracy: %.3f" % scores[1])
        print()


# optional
# visual representation of grid search
# uses seaborn heatmap, could probably do this in matplotlib
import seaborn as sns

sns.set()

train_accuracy = np.zeros((len(eta_vals), len(lmbd_vals)))
test_accuracy = np.zeros((len(eta_vals), len(lmbd_vals)))

for i in range(len(eta_vals)):
    for j in range(len(lmbd_vals)):
        DNN = DNN_keras[i][j]

        train_accuracy[i][j] = DNN.evaluate(X_train, Y_train)[1]
        test_accuracy[i][j] = DNN.evaluate(X_test, Y_test)[1]
```

```
fig, ax = plt.subplots(figsize = (10, 10))
sns.heatmap(train_accuracy, annot=True, ax=ax, cmap="viridis")
ax.set_title("Training Accuracy")
ax.set_ylabel("$\eta$")
ax.set_xlabel("$\lambda$")
plt.show()

fig, ax = plt.subplots(figsize = (10, 10))
sns.heatmap(test_accuracy, annot=True, ax=ax, cmap="viridis")
ax.set_title("Test Accuracy")
ax.set_ylabel("$\eta$")
ax.set_xlabel("$\lambda$")
plt.show()
```

And using PyTorch (more discussions to follow)

```
# Simple neural-network (NN) code using pytorch
import numpy as np
import torch
import torch.nn as nn
import torch.optim as optim

# load the dataset, split into input (X) and output (y) variables
dataset = np.loadtxt('yourdata.csv', delimiter=',')
X = dataset[:,0:8]
y = dataset[:,8]

X = torch.tensor(X, dtype=torch.float32)
y = torch.tensor(y, dtype=torch.float32).reshape(-1, 1)

# define the model
class NNClassifier(nn.Module):
    def __init__(self):
        super().__init__()
        self.hidden1 = nn.Linear(8, 12)
        self.act1 = nn.ReLU()
        self.hidden2 = nn.Linear(12, 8)
        self.act2 = nn.ReLU()
        self.output = nn.Linear(8, 1)
        self.act_output = nn.Sigmoid()

    def forward(self, x):
        x = self.act1(self.hidden1(x))
        x = self.act2(self.hidden2(x))
        x = self.act_output(self.output(x))
        return x

model = NNClassifier()
print(model)

# train the model
loss_fn   = nn.BCELoss()  # binary cross entropy
optimizer = optim.Adam(model.parameters(), lr=0.001)
n_epochs = 100
batch_size = 10

for epoch in range(n_epochs):
    for i in range(0, len(X), batch_size):
        Xbatch = X[i:i+batch_size]
        y_pred = model(Xbatch)
        ybatch = y[i:i+batch_size]
        loss = loss_fn(y_pred, ybatch)
        optimizer.zero_grad()
        loss.backward()
        optimizer.step()

# compute accuracy
y_pred = model(X)
accuracy = (y_pred.round() == y).float().mean()
print(f"Accuracy {accuracy}")

# make class predictions with the model
predictions = (model(X) > 0.5).int()
for i in range(5):
    print('%s => %d (expected %d)' % (X[i].tolist(), predictions[i], y[i]))
```