

INTRODUCTION TO MACHINE LEARNING METHODS

Toni Šćulac Faculty of Science, University of Split, Croatia Corresponding Associate, CERN

tCSC Machine Learning 2024, Split, Croatia



LECTURES OUTLINE

- 1) Introduction to Statistics
- 2) Statistics and Machine Learning
- 3) Classical Machine Learning
- 4) Introduction to Deep Learning
- 5) Advanced Deep Learning



INTRODUCTION TO DEEP LEARNING

*inspiration and examples from <u>3B1B</u> and <u>S. Zhang</u>



NEURAL NETWORKS

- Originate from attempts to model neural processes
- The input is a real number, and the output of each neuron is computed by some non-linear function of the sum of its inputs.
- Neurons typically have a weight that adjusts as learning proceeds. The weight increases or decreases the strength of the signal at a connection.
- Neurons are aggregated into layers. Different layers may perform different transformations on their inputs.
- \odot Can be viewed as a specific way of parametrising transformation functions $\Phi(x)$
 - transformation functions are usually called activation functions





DATASHEET

 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I
 I

Machine learning demystified

BLA Machine Le A BDT Neural Networks - - + - - - + -1.1



NEURAL NETWORKS

- of biological neural networks in animal brains.
- Neurons (or nerve cells) are electrically excitable cells able to fire electric signals across a neural network
- Collects inputs (x_1, \dots, x_N) from other neurons using **dendrites**
- Gathers all the inputs, and fires an electric signal if some conditions are met
- The fired signal is then sent to other neurons through the axon
- Our brain is an extremely large interconnected network of neurons that processes huge amounts of data and tries to model the World





ARTIFICIAL NEURAL NETWORKS

- Why not copy nature? Let's try to build the same thing, but in python (c++)... • Keeping in mind our goal of approximating the LR
- Let's start simple, by designing an artificial Neural Network with:

③ 3 input nodes:

- to keep it real simple in the beginning, let's limit ourselves to 0-1 input
- strength of input signal is modelled by weights

1 neuron:

• we will mimic electric signal of a neuron with an activation function

1 output:

just like in DT it can be 0(b) or 1(s)





PERCEPTRON

- inputs and decides if neuron will fire an electrical signal (1) or not (0)
- Binary output:



• Perceptron is a simple neuron with a simple activation function that aggregates





SIGMOID NEURON

- Small change in weights will result in a small change in output
- Sigmoid functions are a class of functions that resemble shape "S"
- Let's try to build our first NN with a logistic sigmoid function!



Sigmoid neuron uses a sigmoid function that provides a smoother output

$$f(\sum_{i} w_i x_i) = \frac{1}{1 + e^{-\sum_{i} w_i x_i}}$$





layer single-neuron NN that can learn the model behind it:

	X 1	
data 1	0	
data 2	1	
data 3	1	
data 4	0	

- Can your NN
 figure out the model Y(X)?
- Alright, we have the dataset that we will feed to the network and we have figure out how to get our NN to learn from input data!

• Let's define a very simple training dataset and see if we can build a single-



chosen our activation function. Let's plug in some numbers and see if we can



• We need to also choose some starting values for weights

• why not $\vec{w} = (-0.2, 0.4, -1.0)$

Plugging in numbers we get:



• How would you use this information to train your NN?

		X 1	X 2	X 3	Y(x)	Ŷ(
	data 1	0	0	1	0	0.2
.269	data 2	1	1	1	1	0.3
	data 3	1	0	1	0	0.2
	data 4	0	1	1	1	0.3





BACKPROPAGATION

- I think we all agree on the steps of the basic NN learning algorithm:
 - 1. Based on all input data and starting weights calculate the predicted output $\hat{y}(\vec{x}, \vec{w})$
 - 2. Define some kind of a loss (cost) function that is a function of real output values that are known from train data and predicted output $L(y, \hat{y})$
 - 3. Determine how you can change the weights so that the loss function would decrease in value
 - 4. Update weights
 - 5. Repeat steps 1-4 until loss (cost) function can't be reduced anymore
- This procedure is called backpropagation because we are propagating information in the opposite direction of the neural network
- [Fun fact] Biological neural backpropagation is proven to exist but its function remains mysterious.





LOSS FUNCTION

- Loss = measure of misclassification

•
$$L(\vec{x}, \vec{w}) = \frac{1}{2} \sum_{i} \left(y_i - \hat{y}(\vec{x}_i, \vec{w}_i) \right)$$

- \bullet be careful, here index *i* goes over training data (in our case i = 1, 2, 3, 4)
- It is obvious that the training should finish when the loss function is at its minimum
 - The idea is to take repeated steps in the opposite direction of the gradient of the function at the current point, because this is the direction of steepest descent.

• Next step is to define a loss function that measures the error of our estimate

• Many different possibilities, but let's start with a very simple and intuitive one:









GRADIENT DESCENT

- From definition of a gradient we can conclude: • $w_j(t+1) = w_j(t) - \eta \frac{\partial L}{\partial w_i}(t)$
 - where t indicates the index of the iteration of training (epoch) and η is a free parameter called the **learning rate**
- This is where we realise that in order to apply gradient descent our activation function has to be differentiable!

•
$$L(\vec{w}) = \frac{1}{2} \sum_{i} \left(y_i - \hat{y}(\vec{x}_i, \vec{w}_i) \right)^2; \hat{y}(\vec{x}, \vec{w}) = \sigma(\vec{x}, \vec{w}) = \frac{1}{1 + e^{-\vec{w} \cdot \vec{x}}}$$
$$\frac{\partial L}{\partial x} = -\sum_{i} \left[y - \sigma(\vec{w} \cdot \vec{x}) \right] \cdot \left[\sigma(\vec{w} \cdot \vec{x}) (1 - \sigma(\vec{w} \cdot \vec{x})) \right] x_i$$

•
$$\frac{\partial L}{\partial w_j} = -\sum_i [y - \sigma(\vec{w} \cdot \vec{x})] \cdot [\sigma(\vec{w} \cdot \vec{x})]$$



GRADIENT DESCENT

- $\frac{\partial L}{\partial w_i} = -\sum_i [y \sigma(\vec{w} \cdot \vec{x})] \cdot [\sigma(\vec{w} \cdot \vec{x})(1 \sigma(\vec{w} \cdot \vec{x}))]x_j$ • $w_j(t+1) = w_j(t) - \eta \frac{\partial L}{\partial w_i}(t)$
- In our simple example, taking learning rate to be $\eta = 1.0$ at the moment:

•
$$\frac{\partial L}{\partial w_1}(0) = (0110) \begin{pmatrix} -0.053\\ 0.148\\ -0.041\\ 0148 \end{pmatrix} = 0.106$$

- $w_1(1) = w_1(0) + \eta \cdot 0.106; w_1(1) = -0.094$
- $\overrightarrow{w}(0) = (-0.2, 0.4, -1.0) \rightarrow \overrightarrow{w}(1) = (-0.094, 0.695, -0.799)$
- $L(\overrightarrow{w}(0)) = 0.51 \rightarrow L(\overrightarrow{w}(1)) = 0.38$





- We just trained one epoch of a single-layer single-neuron by hand!
 - It is a great achievement, but now it is time to hire python and speed things up
- \bullet We can decide if neuron output is >0.5 the prediction is 1, otherwise it is 0.
- Let's see what happens after 100 epochs!

(base) Tonis-MacBook-Air:Lectures tsculac\$ python SingleNeuron.py For test data [[1 1 0]] NN prediction is [0.98801299] (base) Tonis-MacBook-Air:Lectures tsculac\$

• Success!

• Or is it? How can we make sure the NN learned the correct model?

(base) Tonis-MacBook-Air:Lectures tsculac\$ python For test data [[1 1 0]] NN prediction is [0.9880129 (base) Tonis-MacBook-Air:Lectures tsculac\$ python For test data [[0 0 0]] NN prediction is [0.5] (base) Tonis-MacBook-Air:Lectures tsculac\$

What happened? How can we fix the problem?



-bash	~ະສ1
SingleNeuron.py 99] SingleNeuron.pv	



INTRODUCING BIAS

- move
- This motivates the introduction of a bias term as one input node to our neuron



• We want to guess initial bias and later update it in training

• Having only 0 as input is tricky, because our NN gets stuck and it can never







GRADIENT DESCENT WITH BIAS

• First we need to update the loss function: • $L(\overrightarrow{w}, b) = \frac{1}{2} \sum_{i} \left(y_i - \hat{y}(\overrightarrow{x}_i, \overrightarrow{w}_i, b) \right)^2; \hat{y}(\overrightarrow{x}_i, \overrightarrow{w}_i, b)$ • $\frac{\partial L}{\partial w_i} = -\sum_i \left[y - \sigma(\vec{w} \cdot \vec{x} + b) \right] \cdot \left[\sigma(\vec{w} \cdot \vec{x} + b) \right]$ • $\frac{\partial L}{\partial b} = -\sum_{i} \left[y - \sigma(\vec{w} \cdot \vec{x} + b) \right] \cdot \left[\sigma(\vec{w} \cdot \vec{x} + b) \right]$ • $w_j(t+1) = w_j(t) - \eta \frac{\partial L}{\partial w_i}(t)$ • $b(t+1) = b(t) - \eta \frac{\partial L}{\partial h}(t)$

Time to go back and retrain our NN with bias!

$$\vec{x}, \vec{w}, b) = \sigma(\vec{x}, \vec{w}, b) = \frac{1}{1 + e^{-\vec{w}\cdot\vec{x}+b}}$$

$$(\vec{x} + b)(1 - \sigma(\vec{w} \cdot \vec{x} + b))]x_j$$

$$(\vec{x} + b)(1 - \sigma(\vec{w} \cdot \vec{x} + b))]$$



• Let's define NN parameters: • N_epoch = 100, $\vec{w}(0) = (-0.2, 0.4, -1.0), b(0) = -5, \eta = 0.1$

(base) Tonis-MacBook-Air:Lectures tsculac\$ python SingleNeuron.py For test data [[0 0 0]] NN prediction is [0.00720712] (base) Tonis-MacBook-Air:Lectures tsculac\$

- Success!
- Or is it? How can we make sure the NN learned the correct model?
 - No! We can't just test it on 1 example and call it a day!
 - We need to make a thorough study on more test data
 - We need to see what is happening to the loss/cost function as well!
- In our case, we have 4 test data points that are not part of training: \bullet [0,0,0], [0,1,0], [1,0,0], [1,1,0]





TESTING A NN













TESTING A NN



Single Neuron Network Predicting output that is equal to the value in the second column Test data [[1 1 0]]









SIMPLE NN OVERVIEW

- Building a simple NN from scratch helps us understand key concepts:
 - Input nodes, layers, neurons, outputs
 - Activation functions
 - Backpropagation
 - Loss/cost functions
 - Gradient descent
 - Bias input nodes, learning rate, epochs
 - Training
 - Testing
- We will continue by coming back to some of the above mentioned concepts and discussing how they affect NN and different approaches
- This will give us a deep understanding to be able to move to deep learning





ACTIVATION FUNCTIONS

- neuron fires
- If we want to apply Gradient descent it needs to be differentiable Some common choices that we didn't mention:



It determines at what threshold the neuron will fire or the frequency at which a

Leaky ReLU $\max(0.1x, x)$



Maxout $\max(w_1^T x + b_1, w_2^T x + b_2)$ ELU $\begin{cases} x & x \ge 0 \\ \alpha(e^x - 1) & x < 0 \end{cases}$

*LU = Linear Unit (commonly used for for regression)





UNIVERSAL APPROXIMATION THEOREM

- Neural Networks are extremely powerful because of it \bullet Let σ be any continuous function. The finite sums of the form $G(x) = \sum \alpha_i \sigma(w_i^T x + b_i), \ w_i \in \mathbb{R}^N, \ \alpha_i, b_i \in \mathbb{R} \text{ are dense in } C(\mathbb{R}, \mathbb{R}).$ i=1
 - In other words, given any $\epsilon > 0$ and $f \in C(\mathbb{R}, \mathbb{R})$, there is a sum G(x) of the above form such that $|G(x) - f(x)| < \epsilon, \forall x \in \mathbb{R}^m$
 - The theorem states that for a given function, if there are enough neurons in a NN, then there exists a neural network with that many neurons that does approximate function f to within ϵ
- We solved the problem!
- No : (Theorem does not provide any way to actually find such a sequence. • It also doesn't guarantee any method, such as backpropagation, might actually find such a
 - sequence





GRADIENT DESCENT

- Another commonly used loss function is cross-entropy $L(w,b) = -\sum_{ik} \sum_{k} y_{ik} \log \hat{y}_{ik}$ k
- Choice of learning rate can determine if we get stuck in a local minima or overshoot global minima
 - Output Possible to update (reduce) learning rate as we approach minimal





Just right



STOCHASTIC GRADIENT DESCENT

- this for N epochs
 - this is called batch gradient descent and results in smooth cost vs epoch graph
 - Deep learning uses huge amounts of data so this approach can become extremely slow
- Idea of stochastic gradient descent is to update weights after each event • Mini-batch gradient descent is a combination of 2 that is achieved by
- splitting the training dataset into several smaller ones

Batch gradient descent



• So far we have updated weights averaged over all training cases and repeated

Mini-batch gradient descent

 $\cos t$ $\mathcal{L}_{J(w)}$ Mini-batch #



DEEP NEURAL NETWORK

- Now that we have mastered a single-neuron single-layer NN it is time to move to deep NNs
- "Deep" simply means a lot of hidden layers (and neurons) :)
 - In math language we will move from simple functions that map a couple of real numbers to a single number to extremely complicated functions that map very high-dimensional matrices to some other matrices







ADDING HIDDEN LAYERS

• Let's again start very simple by investigating addition of hidden layers:



- Key element for backpropagation is to calculate the cost/loss function
- We again start simple with cost function of a single training event 0: • $C_0(w^{(1)}, b^{(1)}, w^{(2)}, b^{(2)}, w^{(3)}, b^{(3)}) = (a^{(3)} - y)^2$ • $a^{(3)} = \sigma(z^{(L)}), z^{(3)} = w^{(3)}a^{(2)} + b^{(3)}, a^{(0)} = x$



HIDDEN LAYERS MATH

- $_{\odot}$ We want to understand how a small change in $w^{(3)}$ affects C_0 ?
- Calculus tells us we can figure it out by applying the well known "chain rule"

•
$$\frac{\partial C_0}{\partial w^{(3)}} = \frac{\partial C_0}{\partial a^{(3)}} \frac{\partial a^{(3)}}{\partial z^{(3)}} \frac{\partial z^{(3)}}{\partial w^{(3)}}$$
•
$$\frac{\partial C_0}{\partial a^{(3)}} = 2(a^{(L)} - y), \frac{\partial a^{(3)}}{\partial z^{(3)}} = \sigma'(z(3)), \frac{\partial z^{(3)}}{\partial w^{(3)}} = a^{(2)}$$

 $_{\odot}$ C_0 is the cost function of a single training event. To move to all N events we simply average over all events:

•
$$\frac{\partial C}{\partial w^{(3)}} = \frac{1}{N} \sum_{k=0}^{N-1} \frac{\partial C_k}{\partial w^{(3)}}$$



HIDDEN LAYERS MATH

• To apply gradient descent we need the gradient of the cost function:



- Knowing the gradient and defining the learning rates we can update our weights and biases
- Final step is to allow multiple (many) neurons in each layer!

$$f^{(L)}(a^{(L)} - y), \frac{\partial C_0}{\partial b^{(L)}} = 2\sigma'(z^{(L)})(a^{(L)} - y)$$



DEEP NN = MATRIX MULTIPLICATION

- matrix notation
- Let's look at the example with 2 hidden layers:
- Forward propagation:
 - $Z_1 = W_1 \cdot X + B_1$ • $Z_2 = W_2 \cdot A_1 + B_2, A_1 = \sigma(Z_1)$ • $Z_3 = W_3 \cdot A_2 + B_3, A_2 = \sigma(Z_2)$

• Turns out that equations for deep NN look very nice and simple if you use



DEEP NN = MATRIX MULTIPLICATION

- matrix notation
- Let's look at the example with 2 hidden layers:
- **Backpropagation** with $C = |A_3 Y|^2$: • $dZ_3 = 2(A_3 - Y) \circ f'(Z3)$, $\frac{\partial C}{\partial W_3} = dZ_3 \cdot A_2^T$, $\frac{\partial C}{\partial B_3} = dZ_3$ • $dZ_2 = (W_3^T \cdot dZ_3) \circ f'(Z_2), \frac{\partial C}{\partial W_2} = dZ_2 \cdot A_1^T, \frac{\partial C}{\partial B_2} = dZ_2$

* careful not to mix the dot product (\cdot) and Hadamard product (\circ)

• Turns out that equations for deep NN look very nice and simple if you use

• $dZ_1 = (W_2^T \cdot dZ_2) \circ f'(Z_1), \frac{\partial C}{\partial W_1} = dZ_1 \cdot X^T, \frac{\partial C}{\partial B_1} = dZ_1$



DEEP NN = MATRIX MULTIPLICATION

- matrix notation
- Let's look at the example with 2 hidden layers:
- Update weights and biases:

$$W_1(t+1) = W_1(t) - \eta \frac{\partial C}{\partial W_1}, B_1(t+1) = B_1(t) - \eta \frac{\partial C}{\partial B_1}$$

$$W_2(t+1) = W_2(t) - \eta \frac{\partial C}{\partial W_2}, B_2(t+1) = B_2(t) - \eta \frac{\partial C}{\partial B_2}$$

$$W_3(t+1) = W_3(t) - \eta \frac{\partial C}{\partial W_3}, B_3(t+1) = B_3(t) - \eta \frac{\partial C}{\partial B_3}$$

• Turns out that equations for deep NN look very nice and simple if you use



- ourselves?
- **MNIST** data



- We will take 70k 28x28 pixel images
- For each pixel there is a value 0-255 indicating its value on grayscale (0=black, 255=white)
- Each picture comes with a 0-9 label

• Did we really understand deep NNs if we don't code these matrix equations

• Let's try building a NN that can recognise handwritten digits from the famous



- We simply choose a NN with 28x28=784 input neurons
- We add 2 hidden layers with 16 neurons in each one
- Output layer has 10 neurons (idea is that each one carries information on how likely the number corresponds to that digit)



16





• Let's define our matrices and their dimensions:







• We are ready to turn this math into python code!

```
def init_NN_parameters():
    w1 = np.random.rand(16,28*28)-0.5
    b1 = np.random.rand(16,1)-0.5
    w^2 = np.random.rand(16, 16) - 0.5
    b2 = np.random.rand(16,1)-0.5
   w3 = np.random.rand(10, 16) - 0.5
    b3 = np.random.rand(10,1)-0.5
    return w1,b1,w2,b2,w3,b3
```

```
def back_propagation(X,Y, Z1,A1,Z2,A2,Z3,A3,w2,w3):
    m = Y.size
    dZ3 = 2*(A3 - Y)*der_ReLU(Z3)
    dW3 = (1/m) * dZ3.dot(A2.T)
    dB3 = (1/m) * np.sum(dZ3,1)
    dZ2 = w3.T.dot(dZ3)*der_ReLU(Z2)
    dW2 = (1/m) * dZ2.dot(A1.T)
    dB2 = (1/m) * np.sum(dZ2,1)
    dZ1 = w2.T.dot(dZ2)*der_ReLU(Z1)
    dW1 = (1/m) * dZ1.dot(X.T)
    dB1 = (1/m) * np.sum(dZ1,1)
    return dW3,dB3,dW2,dB2,dW1,dB1
```

```
def forward_propagation(X, w1,b1,w2,b2,w3,b3):
    Z1 = w1.dot(X) + b1
   A1 = ReLU(Z1)
    Z2 = w2.dot(A1) + b2
   A2 = ReLU(Z2)
   Z3 = w3.dot(A2) + b3
   A3 = ReLU(Z3)
    return Z1,A1,Z2,A2,Z3,A3
```

```
def update_params(alpha, w3,b3,w2,b2,w1,b1,dW3,dB3,dW2,dB2,dW1,dB1):
    w3 = w3 - alpha * dW3
    b3 = b3 - alpha*dB3.reshape(10,1)
    w2 = w2 - alpha * dW2
    b2 = b2 - alpha * dB2.reshape(16,1)
    w1 = w1 - alpha * dW1
    b1 = b1 - alpha*dB1.reshape(16,1)
    return w3,b3,w2,b2,w1,b1
```





• We decide to split our dataset into 60k training points and 10k test points. Training it for 1500 epochs with 0.1 learning rate:

```
Epoch 0
[7 6 7 ... 5 6 7] [5 0 4 ... 5 6 8]
Accuracy 0.118316666666666667
Cost function = 279650.33817947295
Epoch 50
[9 0 4 ... 5 6 8] [5 0 4 ... 5 6 8]
Accuracy 0.263
Cost function = 68318.50986350718
Epoch 100
[5 0 4 ... 5 6 8] [5 0 4 ... 5 6 8]
Accuracy 0.35961666666666666
Cost function = 57361.1053264526
```

```
Epoch 1400
[5 0 4 ... 5 6 8] [5 0 4 ... 5 6 8]
Accuracy 0.734933333333333333
Cost function = 26348.145017085022
Epoch 1450
[5 0 4 \dots 5 6 8] [5 0 4 \dots 5 6 8]
Accuracy 0.7387
Cost function = 26018.279174079744
Epoch 1499
[5 0 4 ... 5 6 8] [5 0 4 ... 5 6 8]
Accuracy 0.742033333333333333
Cost function = 25708.492532038963
```

Don't forget to check for overtraining

[7 2 1 ... 4 8 6] [7 2 1 ... 4 5 6] Accuracy on test data 0.7494







- Not a bad performance for numpy only deep NN!
- [CHALLENGE] Can you beat me? Can you write a better deep NN to solve the same problem using only NumPy?



Prediction: [9] Label: 2









CONCLUSIONS AND OUTLOOK

- Machine Learning is only a powerful tool in the hands of someone who understands how it works
- It is impossible to fully understand every single detail of what happens inside of a multilayered NN/BDT
 - But that doesn't mean you can't fully understand the concept and mathematics behind it and be able to apply it in a simplified version
- Everything we have discussed so far is considered Classical (old) Machine Learning and is not even close in performance with State of the Art
 - However, all the concepts that we have learned about are the key of modern ML
- In the reminder of the school you will learn about state of the art ML and its application to HEP
 - Whenever things seem to be too complicated to understand, just drop back to basics and try to understand it in an overly simplified version like we did together





