Introduction to Machine Learning: Part I

Prof. Sean Dobbs[1] & Daniel Lersch[2]

April 16, 2020

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About this Lecture

- **Part I:**
  - Introduction to DataFrames
  - Basic concepts of machine learning
    (with focus on feedforward neural networks)
- **Part II:**
  - Machine learning in (physics) data analysis
  - Performance evaluation
- **Part III:**
  - Algorithm tuning
  - Hyper parameter optimization
- **Part IV:**
  - Custom neural networks with Tensorflow
  - Transition to Deep Learning

The individual contents might be subject to change

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... introduce a few machine learning algorithms

... utilize the **scikit-learn** library

... most likely contain several errors ($\rightarrow$ Please send a mail to `dlersch@jlab.org`)

Homework and Literature

- Machine learning can be learned best by simply doing it!

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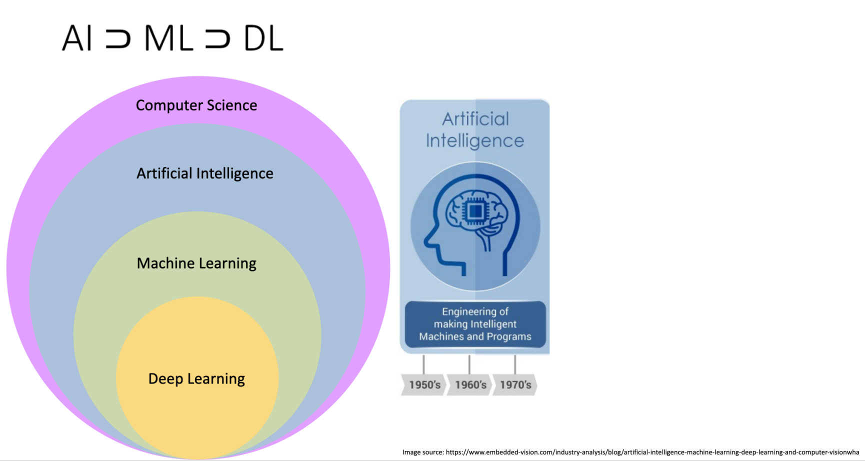
- Helpful literature:
  - The **scikit-learn** documentation
  - Talks from the **deep learning for science school 2019**[3]
  - "Hands-On Machine Learning with Scikit-Learn, Keras & Tensorflow", by Aurélien Géron
  - The internet is full of good (but also very bad!) literature[4] → browse with caution
  - The slides of the lecture are available at: `http://hadron.physics.fsu.edu/~dlersch/ml_slides/`

[3] Very good and detailed explanation of (deep) neural networks

[4] Any document claiming that there is a quick way to understand machine learning without any theory / math is considered as bad

AI, ML and DL



Slide taken from Brenda Ngs introductory talk at the: **deep learning for science school 2019**

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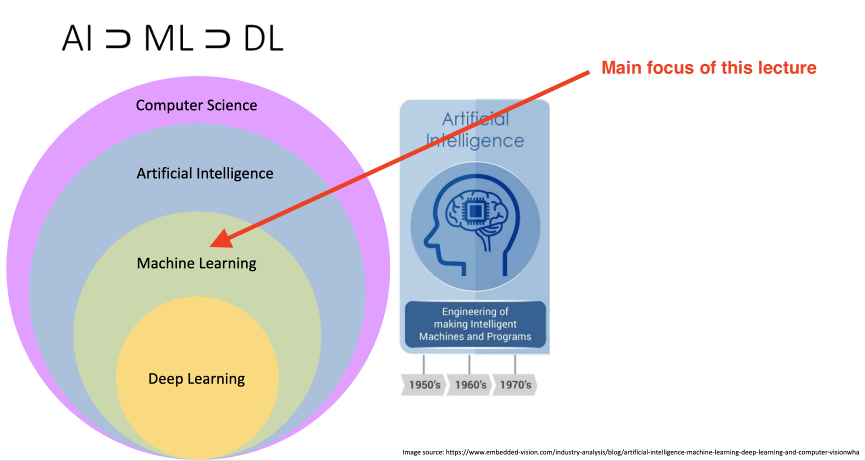

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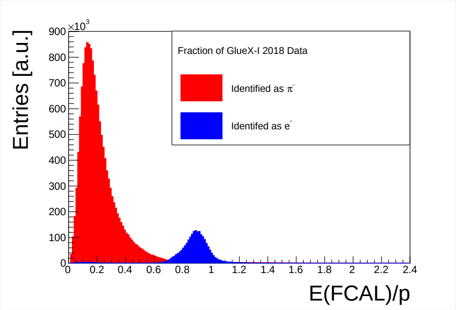

$\Rightarrow$ Particle identification at GlueX

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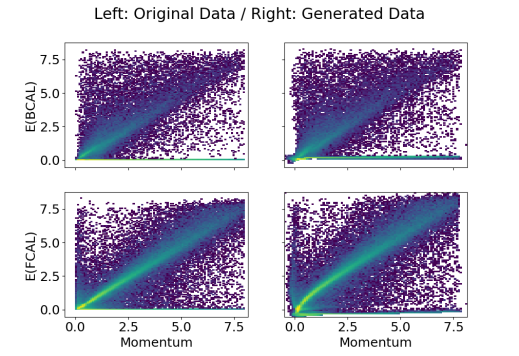
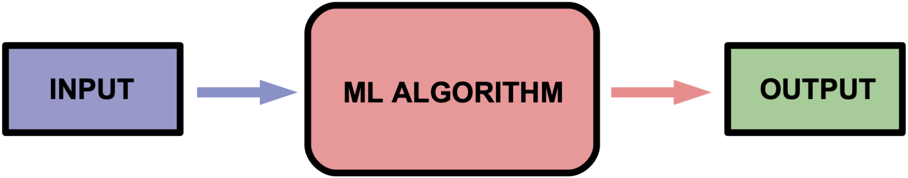


$\Rightarrow$ Simulate particles (leptons) at GlueX

Basic Components of Machine Learning



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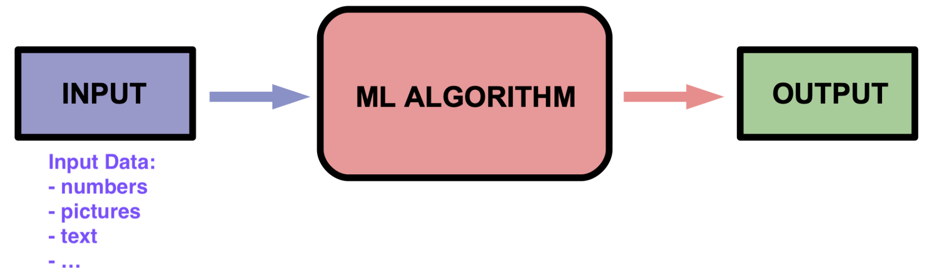

Basic Components of Machine Learning

Input Data:
- **numbers**
- **pictures**
- **text**
- **...**

- **Before passing any data to any algorithm, you might want to take a look at it first**

- **The data (sometimes) requires pre-processing**

—> Need an efficient way to handle (large) data sets —> DataFrames

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0	value(col1,row1)	value(col2,row1)	$\cdots$	value(colN,row1)
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- They may contain multiple data types

  $\rightarrow$ Numbers

	value a	value b
0	0.3	-11.0
1	-1.2	0.8
2	5.0	12.0

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  $\rightarrow$ Text

```
  Language    Hello   My name is          I am hungry
0   French  Bonjour      Je suis   Je suis affame
1   German    Hallo  Ich heisse  Ich habe hunger
```

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⋮	⋮	⋮	⋮	⋮

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  → Text and Numbers

	Student	Points	Comment
0	A	9.9	Dedicated
1	B	10.0	Brilliant
2	C	-100.0	Makes me cry

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  $\rightarrow$ Vectors

	State Vector	Score
0	[0, 1]	0.5
1	[1, 0]	0.5
2	[1, 1]	1.0
3	[0, 0]	0.3

Creating,Loading and Saving DataFrames

- Create a DataFrame from scratch

```python
import pandas as pd
#Define the data:
data = {
    'Col1': [1,2,3],
    'Col2': [ 'a','b','c'],
    'Col3': [True,False,True]
}
#Create the dataframe:
df = pd.DataFrame(data)
#And print it:
print(df)
```

	Col1	Col2	Col3
0	1	a	True
1	2	b	False
2	3	c	True

Creating,Loading and Saving DataFrames

- Create a DataFrame from scratch
- Or load it from a .json, .csv, ... file

```
import pandas as pd
df_1 = pd.read_csv(...)
df_2 = pd.read_json(...)
df_3 = pd.read_pickle(...)
df_4 = pd.read_excel(...)
```

Creating,Loading and Saving DataFrames

- Create a DataFrame from scratch
- Or load it from a .json, .csv, ... file
- After working with your DataFrame, you might want to save it

```
import pandas as pd
df_1.to_csv(...)
df_2.to_json(...)
df_3.to_pickle(...)
df_4.to_excel(...)
```

Creating and Manipulating DataFrames

- Create a DataFrame from numpy arrays

```
import numpy as np
import pandas as pd
#Create 20 data points, having 2 values between -10 and 10 each:
data = np.random.uniform(low=-10,high=10,size=(20,2))
#Turn this 20x2 array into a DataFrame:
df = pd.DataFrame(data)
#And name the two columns:
df.columns = ['Values_1','Value_2']
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```

	Value_1	Value_2
0	-4.433853	5.134270
1	-2.473114	6.353864
2	-3.052877	1.804706
3	6.370931	-1.781364
4	3.368881	-2.075033
5	-1.700772	0.982987
6	-3.453366	-5.401645
7	-0.891402	3.541155
8	6.937076	-9.000622
9	-8.738868	-9.841198
10	4.450625	-5.901079
11	-3.531955	-3.088243
12	6.313612	4.286357
13	1.438309	5.890397
14	-0.451029	4.349020
15	4.185787	6.036617
16	-3.157958	2.286626
17	2.243423	-3.431162
18	-1.778005	6.958256
19	6.502947	-9.102705

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df['Value_3'] = df['Value_2']*2
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3	6.370931	-1.781364	-3.562728
4	3.368881	-2.075033	-4.150066
5	-1.700772	0.982987	1.965973
6	-3.453366	-5.401645	-10.803290
7	-0.891402	3.541155	7.082311
8	6.937076	-9.000622	-18.001244
9	-8.738868	-9.841198	-19.682396
10	4.450625	-5.901079	-11.802157
11	-3.531955	-3.088243	-6.176486
12	6.313612	4.286357	8.572715
13	1.438309	5.890397	11.780794
14	-0.451029	4.349020	8.698039
15	4.185787	6.036617	12.073234
16	-3.157958	2.286626	4.573253
17	2.243423	-3.431162	-6.862324
18	-1.778005	6.958256	13.916511
19	6.502947	-9.102705	-18.205410

Creating and Manipulating DataFrames

- Create a DataFrame from numpy arrays
- Create a third column which is equal to the second column multiplied by 2
- Create a fourth column, based on the first column + a user-defined function

```
#Define your function:
def lin_func(x,m,b):
     return m*x+b
 #Use the lambda function to create a fourth column,
 #based on the values from the first column:
 df['Value_4'] = df['Value_1'].apply(lambda x: lin_func(x,-0.5,3.3))
 #Value_4 = -0.5*Value_1 + 3.3
```

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0	-4.433853	5.134270	10.268539	5.516927
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3	6.370931	-1.781364	-3.562728	0.114535
4	3.368881	-2.075033	-4.150066	1.615560
5	-1.700772	0.982987	1.965973	4.150386
6	-3.453366	-5.401645	-10.803290	5.026683
7	-0.891402	3.541155	7.082311	3.745701
8	6.937076	-9.000622	-18.001244	-0.168538
9	-8.738868	-9.841198	-19.682396	7.669434
10	4.450625	-5.901079	-11.802157	1.074687
11	-3.531955	-3.088243	-6.176486	5.065978
12	6.313612	4.286357	8.572715	0.143194
13	1.438309	5.890397	11.780794	2.580845
14	-0.451029	4.349020	8.698039	3.525515
15	4.185787	6.036617	12.073234	1.207106
16	-3.157958	2.286626	4.573253	4.878979
17	2.243423	-3.431162	-6.862324	2.178288
18	-1.778005	6.958256	13.916511	4.189003
19	6.502947	-9.102705	-18.205410	0.048527

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	Expected Values Col2	Observed Values Col2
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sigma	$20/\sqrt{12} \approx 5.77$	5.61

- You can also access the mean / std. dev. for all DataFrame columns

```
mean_all = df.mean()
sigma_all = df.std()
```

Visualizing DataFrames with pyplot

- Want to plot different columns from the DataFrame
- Histogram the fourth column

```
import matplotlib.pyplot as plt
plt.rcParams.update({'font.size': 18}) #--> Set the font size
plt.hist(df['Value_4'],bins=100) #--> Plot fourth column in 100 bins
plt.xlabel('Value_4')
plt.ylabel('Entries')
plt.show()
```

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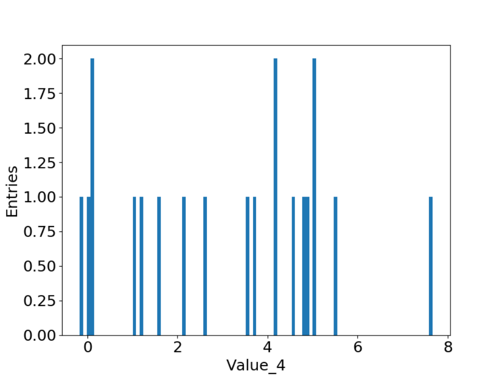

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- Plot correlation between first and fourth column

```
#Define a 2d histogram with 100 bins on each axis
plt.hist2d(df['Value_1'],df['Value_4'],bins=100)
plt.xlabel('Value_1')
plt.ylabel('Value_4')
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```

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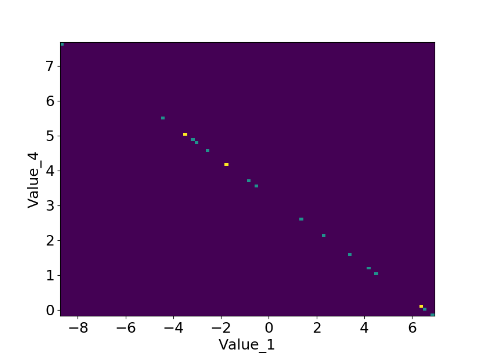
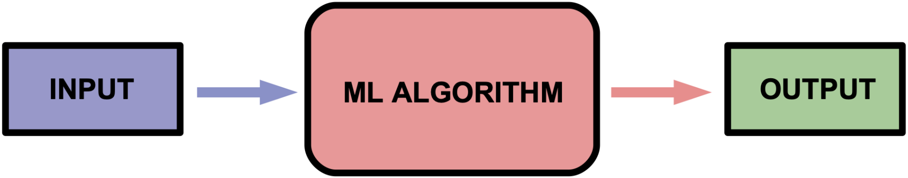


DataFrames: Summary and Outlook

- Introduced DataFrames for convenient data analysis / visualization
- Did NOT show all functionalities
  - Concatenating / stacking DataFrames
  - Shuffling DataFrames
  - ...
- Python provides a detailed documentation about DataFrames and related functions

Basic Components of Machine Learning



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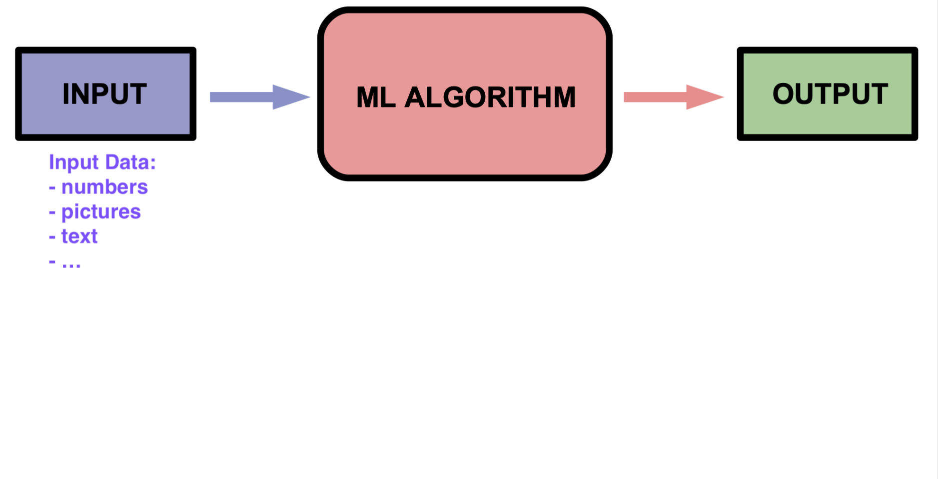

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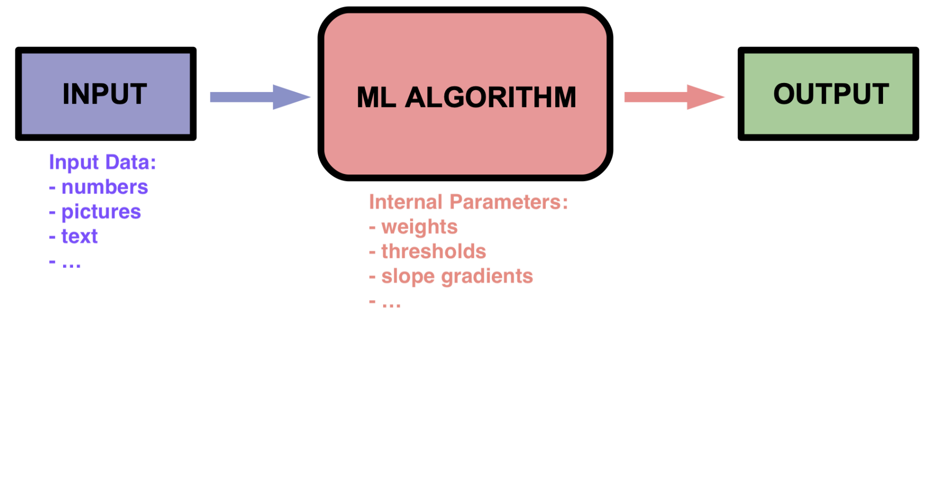

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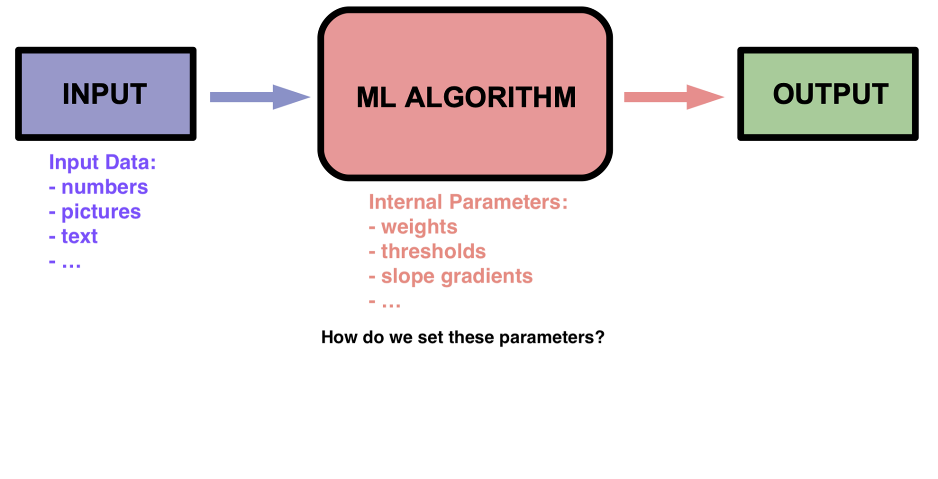

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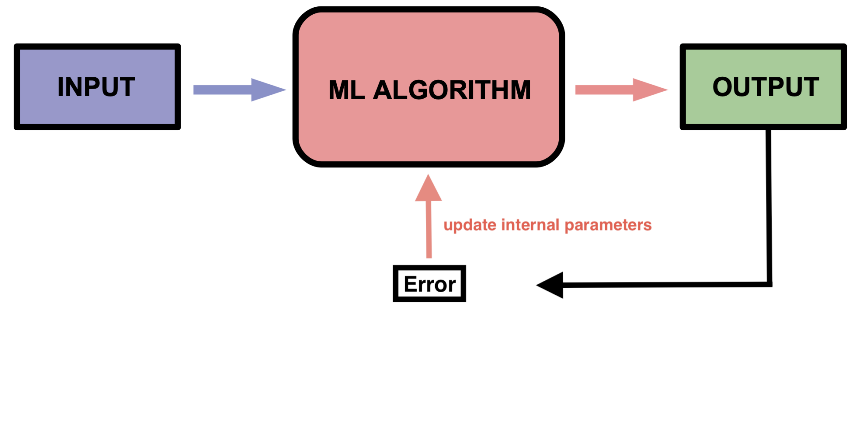

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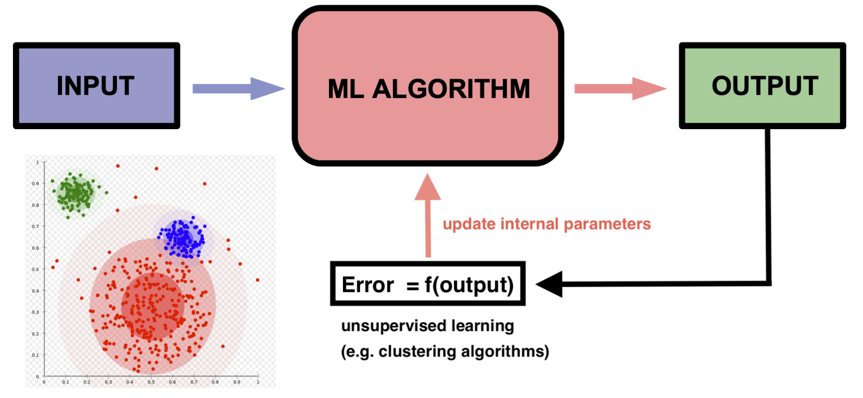

clustering algorithm
taken from: wikipedia
By Chire - Own work, CC BY-SA 3.0, https://commons.wikimedia.org/w/index.php?curid=17087089

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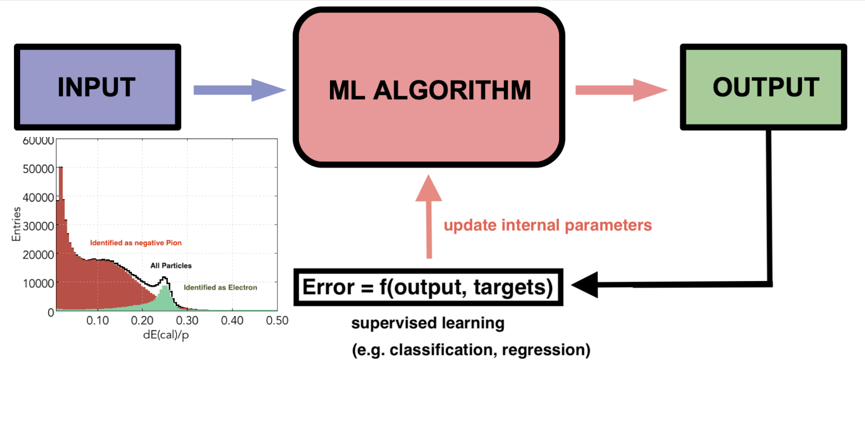

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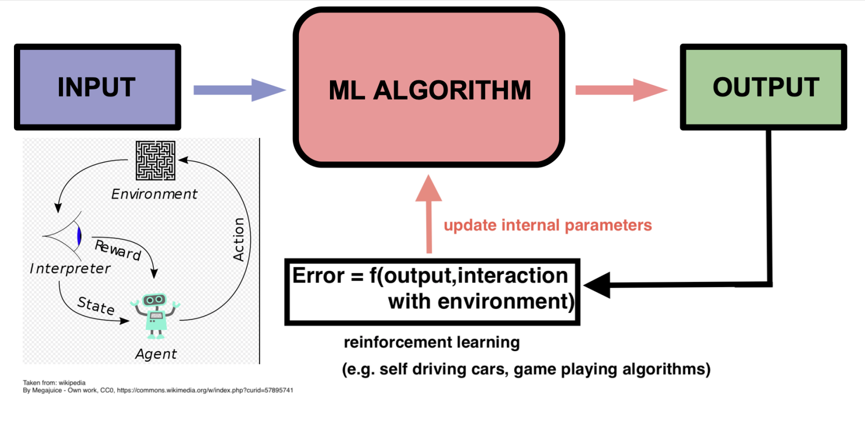

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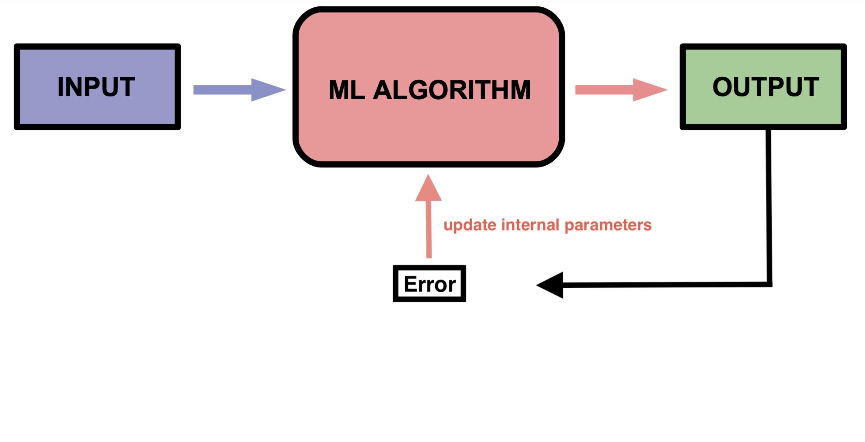

- **Goal:** Minimize error

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- Most important tool to check whether training was successful: **Training Curve**
- The training itself is not difficult, as many frameworks already support the training procedures for a variety of machine learning algorithms
  $\rightarrow$ You do not need to take care of updating the algorithms parameters [5]

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- The training itself is not difficult, as many frameworks already support the training procedures for a variety of machine learning algorithms
  $\rightarrow$ You do not need to take care of updating the algorithms parameters [5]
- **Tricky:** How to set up and evaluate the training properly (will be discussed soon)

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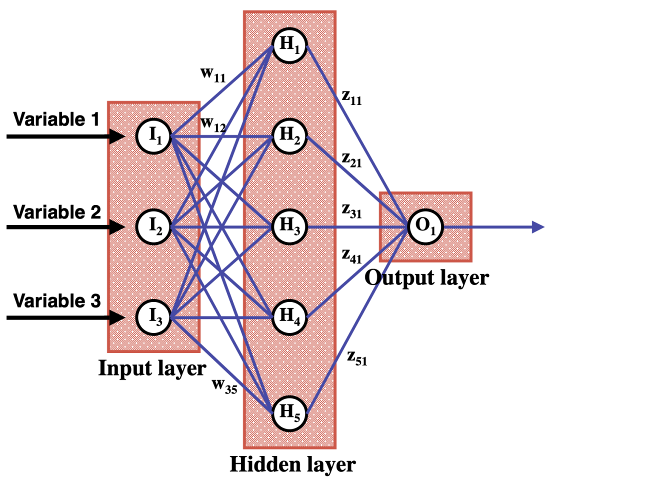
  - Algorithms internal parameters are updated several times
  - Ideally: Error should get smaller with every update
- Most important tool to check whether training was successful: **Training Curve**
- The training itself is not difficult, as many frameworks already support the training procedures for a variety of machine learning algorithms
  $\rightarrow$ You do not need to take care of updating the algorithms parameters [5]
- **Tricky:** How to set up and evaluate the training properly (will be discussed soon)
- **Next:** Discuss training of a feedforward neural network

[5] There are exceptions of course which will be discussed in a later part of this lecture

The Multilayer Perceptron



- Most popular example for machine learning algorithms
- Belongs to the class of feedforward neural networks
- **Architecture:** Hidden layers with a set of neurons

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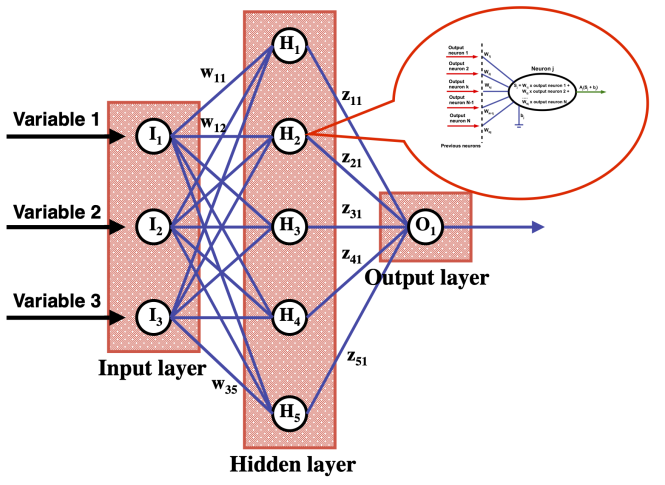

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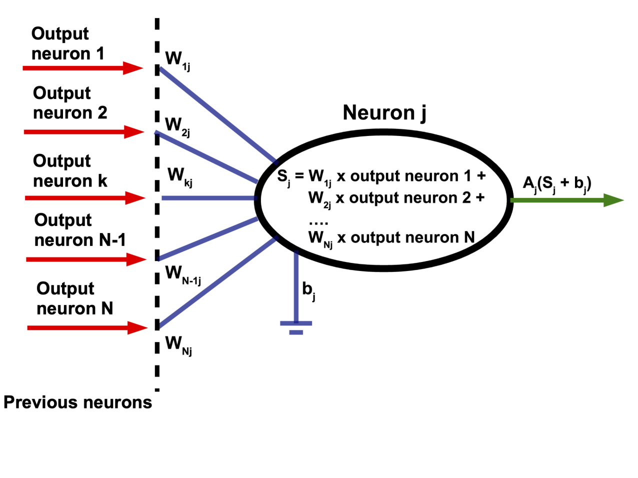

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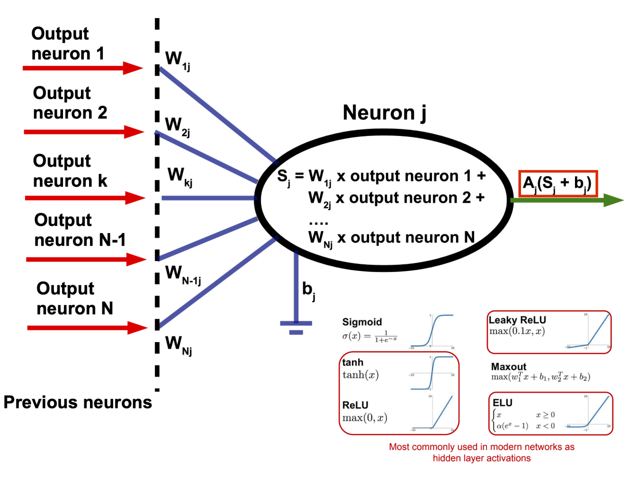

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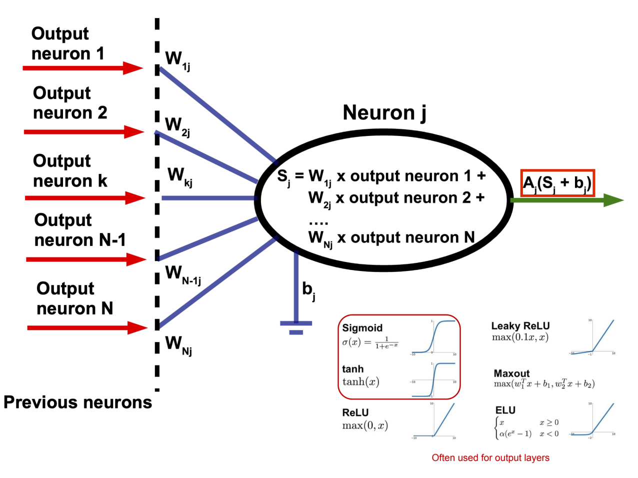

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The Universal Approximation Theorem for Neural Networks

"a single hidden layer neural network with a linear output unit can approximate any continuous function arbitrarily well, given enough hidden units" -- Hornik, 1991,
http://zmjones.com/static/statistical-learning/hornik-nn-1991.pdf

This, of course, does not imply that we have an optimization algorithm that can find such a function. The layer could also be too large to be practical.

$n_1(x) = Relu(-5x - 7.7)$
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$n_4(x) = Relu(1.2x - .2)$
$n_5(x) = Relu(2x - 1.1)$
$n_6(x) = Relu(5x - 5)$

$$Z(x) = -n_1(x) - n_2(x) - n_3(x) + n_4(x) + n_5(x) + n_6(x)$$

Fig. credit towardsdatascience.com/can-neural-networks-really-learn-any-function-65e106617fc6

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$\Rightarrow$ Similarly formulated in 1990 by the **Stone-Weierstrass-Theorem**
"[...] there are no nemesis functions that cannot be modeled by neural networks"

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⇒ Neural networks are powerful tools! But,...

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- How do we set 26 parameters???

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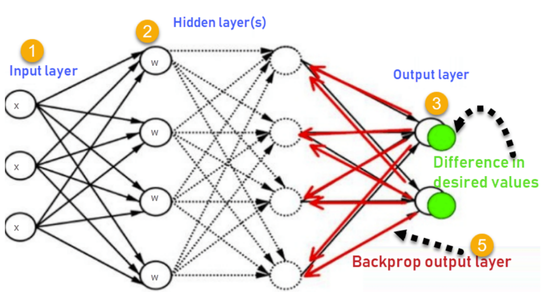
Backpropagation



How Backpropagation Works

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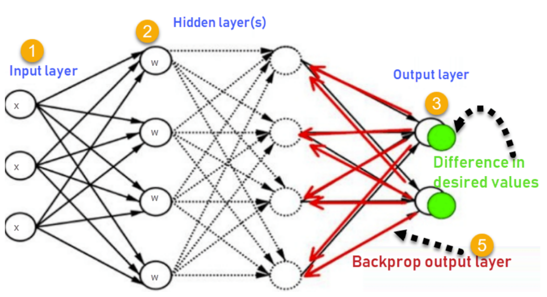

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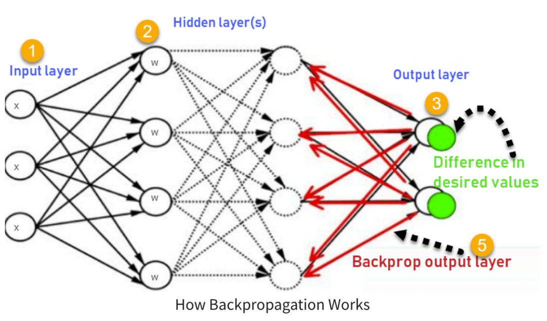

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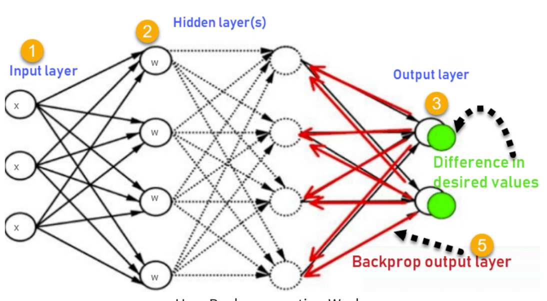

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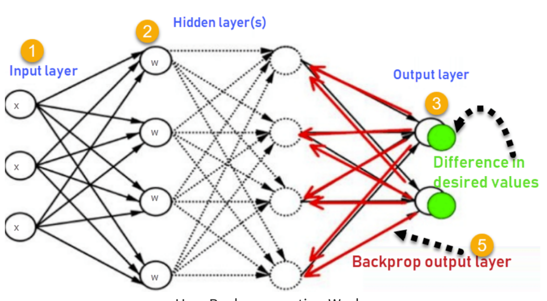

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- Most prominent example: $L = [y_{true} - y_{network}(x_{data}, w_k)]^2$

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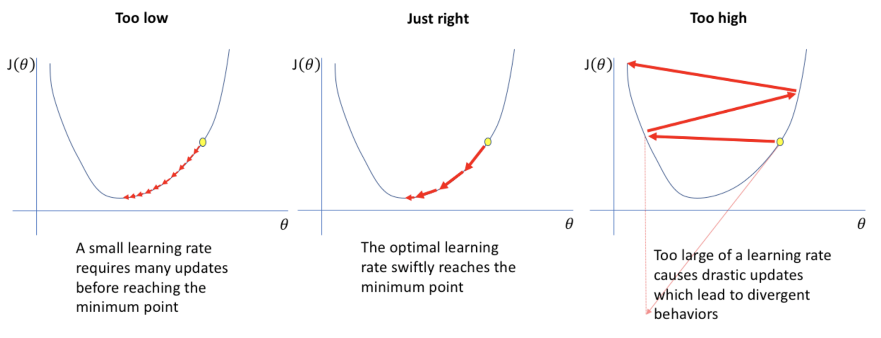

Picture taken form **Jeremy Jordans Blog**

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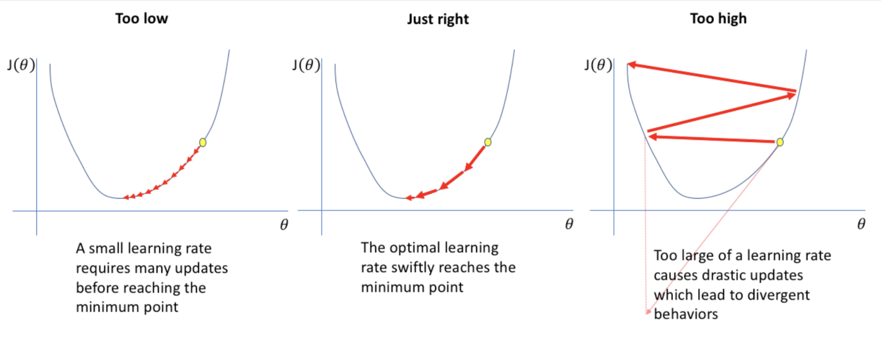

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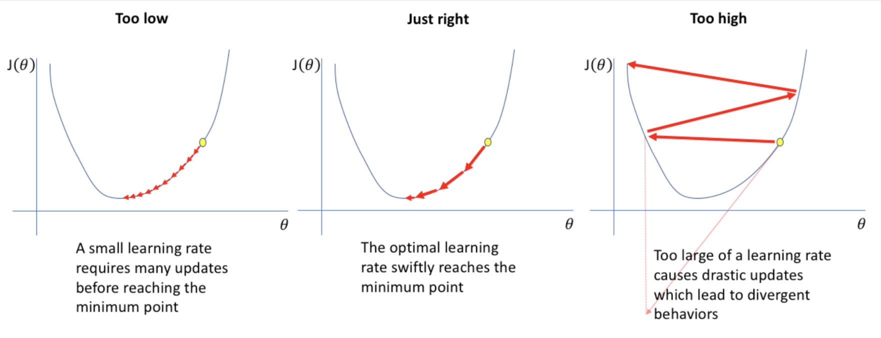

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- **Cost Function J** $= \frac{1}{N} \sum_{\text{entire training data}}$ (**Loss Function L**) + Regularization[7]
- Different algorithms to find minimum of J: Steepest Gradient Descent (SGD), ADAM, Limited memory Broyden-Fletcher-Goldfarb-Shanno algorithm (LBFGS),...

[7] You can think of this as setting constraints to the weights

Example: Learning the Quadratic Function

Setting up the Data Set

- Create the data which shall be learned

```
#Generate 500 (random) x-values between -3 and 3:
x_values = np.random.uniform(low=-3.0,high=3.0,size=(500,1))
#size=(500,1)--> This format is needed for the ml algorithm
#Use the lambda function to get the y-values:
quadratic_func = lambda x: x*x
y_values = quadratic_func(x_values).flatten() #--> needed for ml alg.
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- Plot the data

```
#Visualize the results with the pyplot library:
plt.rcParams.update({'font.size': 18}) #--> Set the fond size
plt.plot(x_values,y_values,'ko') #--> Plot the data as points
plt.xlim((-3,3)) #--> Set limits on x-axis
plt.xlabel('x')
plt.ylabel('f(x)')
plt.show()
```

Example: Learning the Quadratic Function

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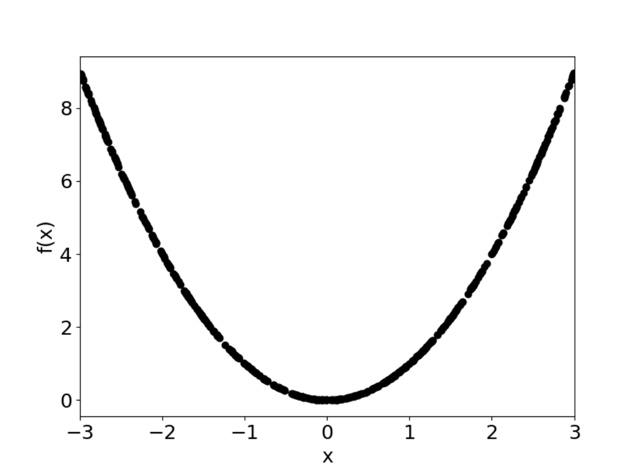

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- Setup the network with scikit

```
#Import the proper library from scikit:
from sklearn.neural_network import MLPRegressor
#Setup the network:
my_mlp =   MLPRegressor(
           hidden_layer_sizes=(10), #one hidden layer with 10 neurons
           activation='relu', #rectified linear unit function
           solver='sgd', #stochastic gradient descent optimizer
           #--> to minimize the error
           warm_start=True,
           max_iter = 500, #maximum  number of learning epochs
           shuffle=True, #shuffle the data
           random_state=0,
           learning_rate_init = 0.05 #step size for the gradient
       )
```

Example: Learning the Quadratic Function

Setting up the Model

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```
#Start training of network, i.e. fit model to the data:
my_mlp.fit(x_values,y_values)
#And get the training curve:
training_curve = my_mlp.loss_curve_
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- Plot the training curve

```
#Plot the training curve:
plt.plot(training_curve,'-',linewidth=2.0)
plt.xlabel('Epoch')
plt.ylabel('Error')
plt.show()
```

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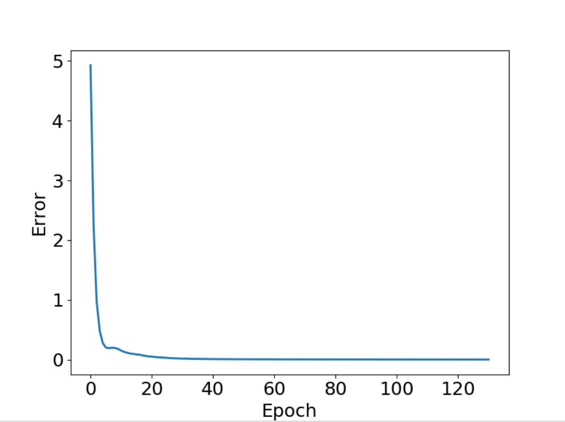

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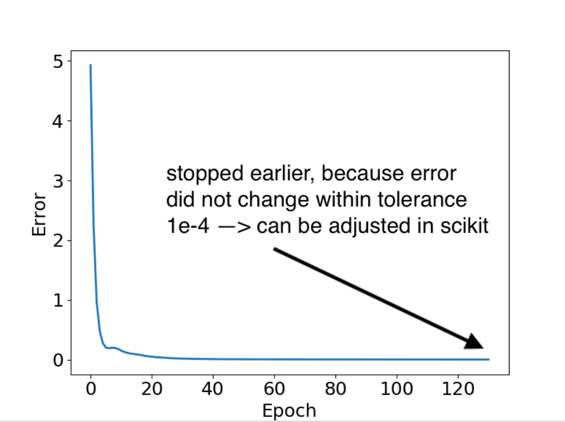
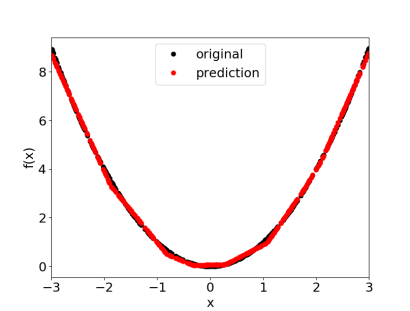


Example: Learning the Quadratic Function

Inspecting the Results



- Model predictions look reasonable so far
- Can do better $\rightarrow$ tune model
- How well does model generalize, i.e. make reasonable predictions on data that has not been used during training

Unknown Value	Model Prediction
-4	14
6	24

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- A very helpful tool to monitor the performance of (any) fit are residuals
- Residual = True Output - Predicted Output

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```
#Define residual function:
residual_func = lambda x,y: x-y
#Apply function on true / predicted values:
residuals = residual_func(y_values,predicted_values)
#And finally plot everything
plt.hist(residuals,bins=50)
plt.xlabel(r'$y_{true} - y_{network}$') #---> Inlcude latex expressions
plt.ylabel('Entries [a.u.]')
plt.show()
```

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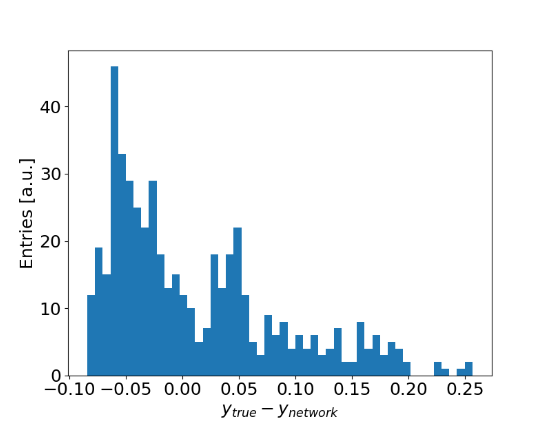

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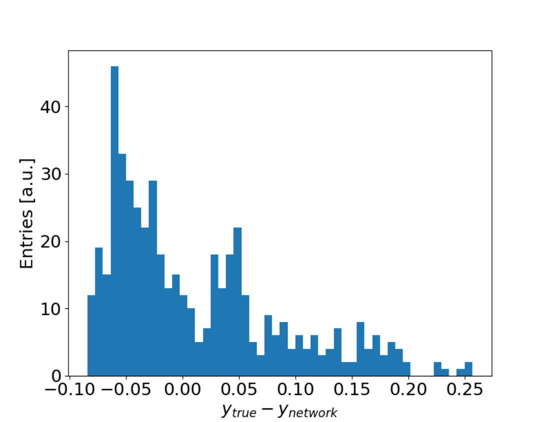

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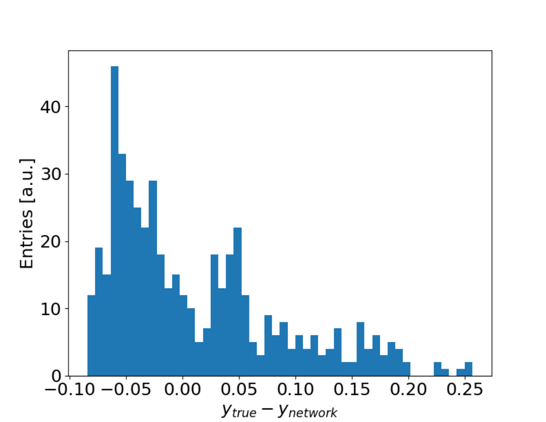

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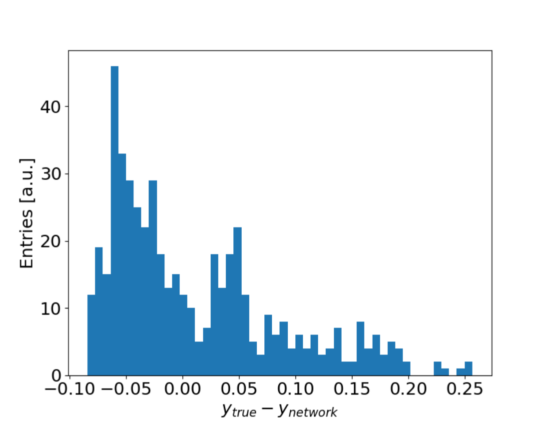

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- **Note:** Did NOT follow best-practice during this example → Will be discussed in part II

Summary Part I

- Introduced DataFrames into analysis
  - Structure data
  - Manipulate data
  - Visualization
- Basic concepts of training a machine learning algorithm
  - Set internal parameters by minimizing error
  - (un-) supervised and reinforcement learning
- Discussed training of a multilayer perceptron in more detail
  - Update weights by minimizing loss
  - Example: Learning a quadratic function