# Introduction to Machine Learning: Part IV

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

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

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

# Homework and Literature

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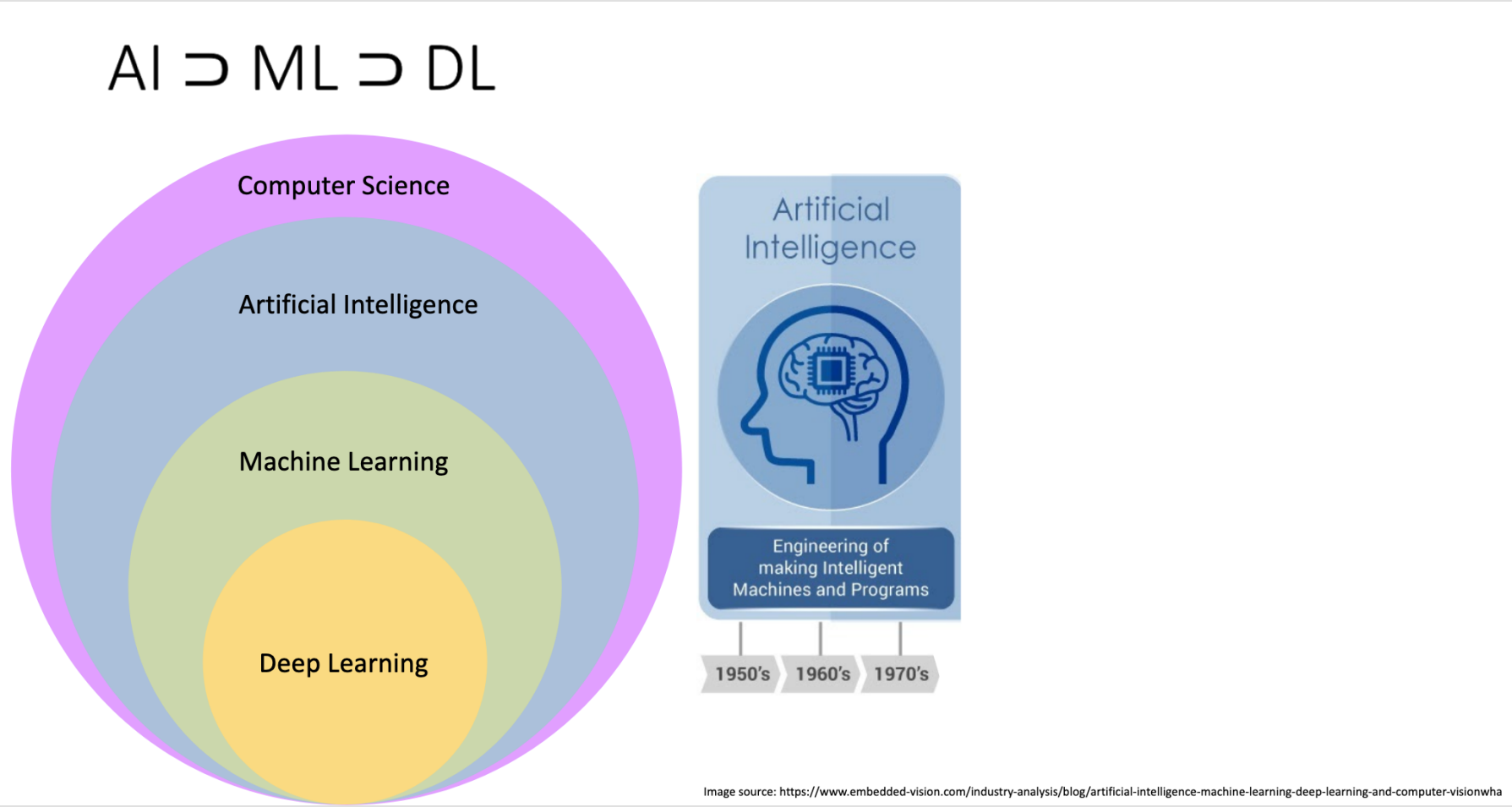
- Helpful literature:
  - The **scikit-learn** documentation
  - Talks from the **deep learning for science school 2019**[3]
  - "Hands-On Machine Learning with Scikit-Learn, Keras & Tensorflow", by Aurélien Géron
  - The internet is full of good (but also very bad!) literature[4] $\rightarrow$ browse 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

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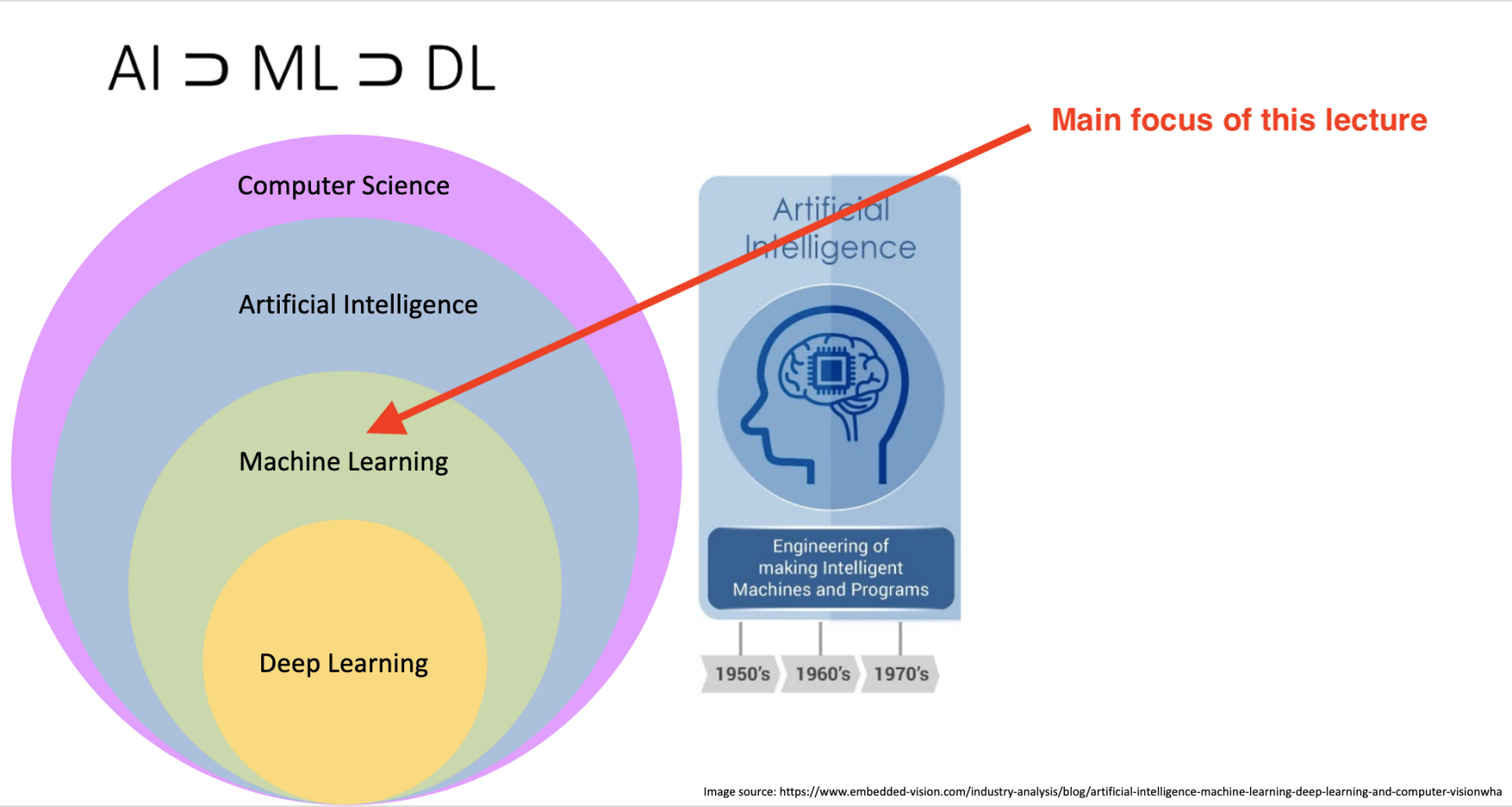


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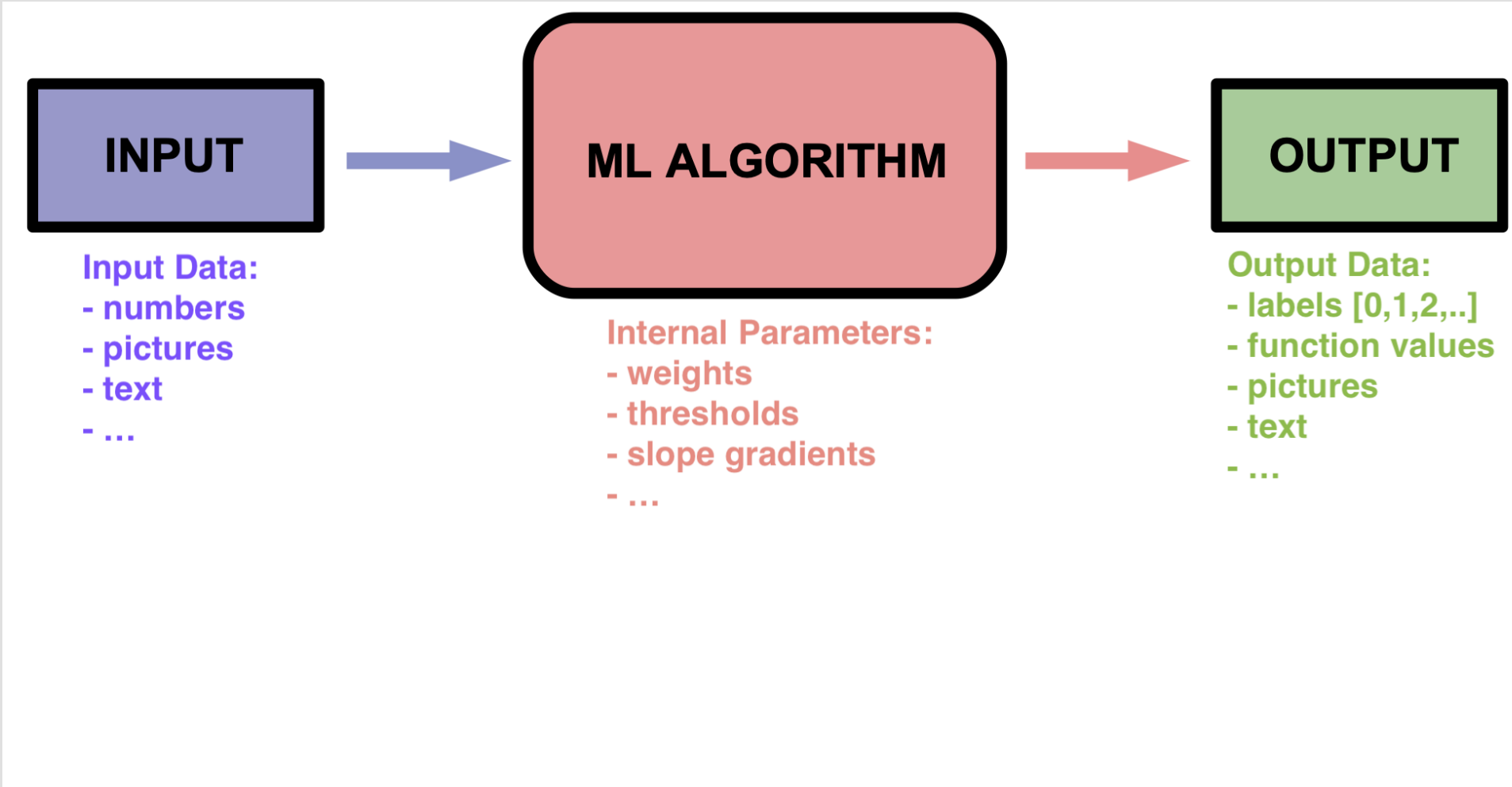
# Basic Components of Machine Learning



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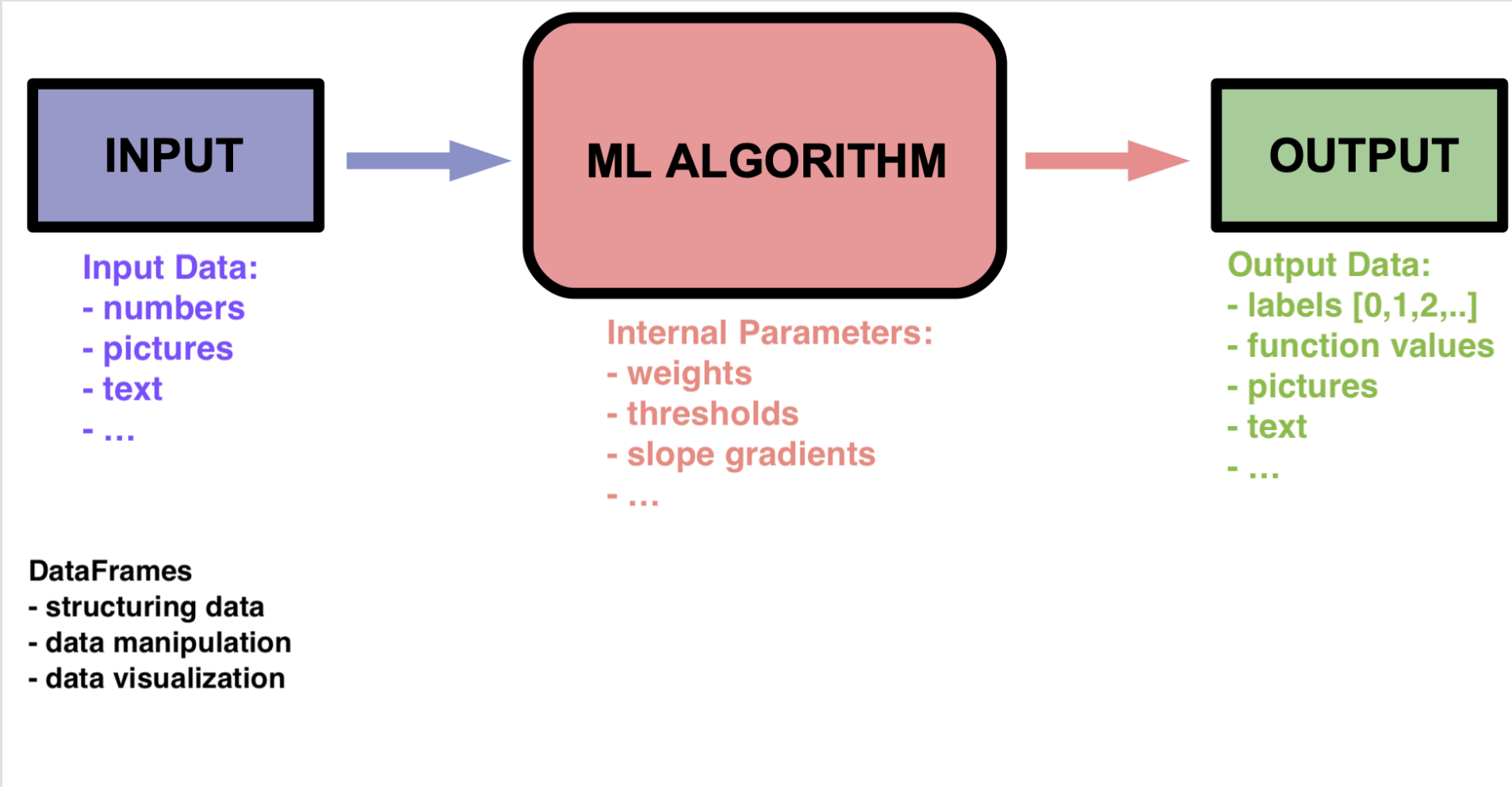

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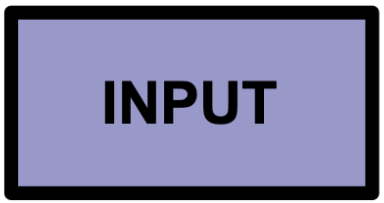


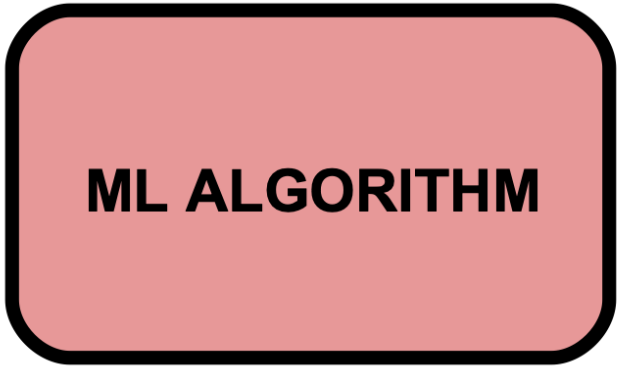


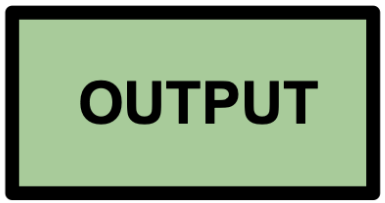


**Input Data:**
- numbers
- pictures
- text
- ...

**Internal Parameters:**
- weights
- thresholds
- slope gradients
- ...

**Output Data:**
- labels [0,1,2,..]
- function values
- pictures
- text
- ...

**DataFrames**
- structuring data
- data manipulation
- data visualization

**algorithm types**
- MLP
- SVM
- Random Forest
- ...

**learning strategies**
- (un) supervised,...
- validation data
- minimization techniques
- HPO

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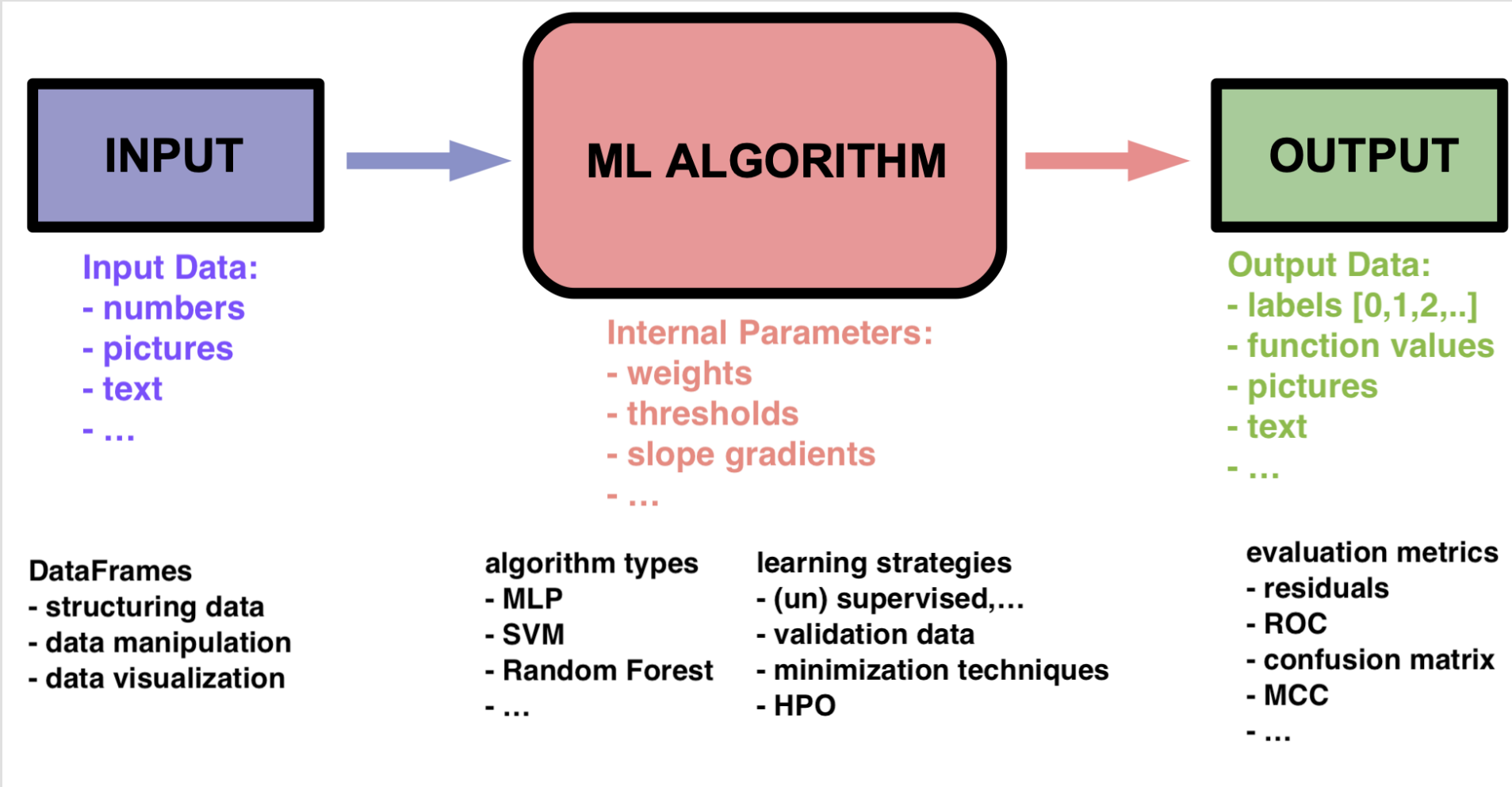

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  - Might have to try many parameter combinations
  - No guarantee that optimum is found
- (One) alternative: try a random walk search
  - Explore parameter space by random selection
  - Add selection rules, e.g. mlp shall grow in depth, rather than in width

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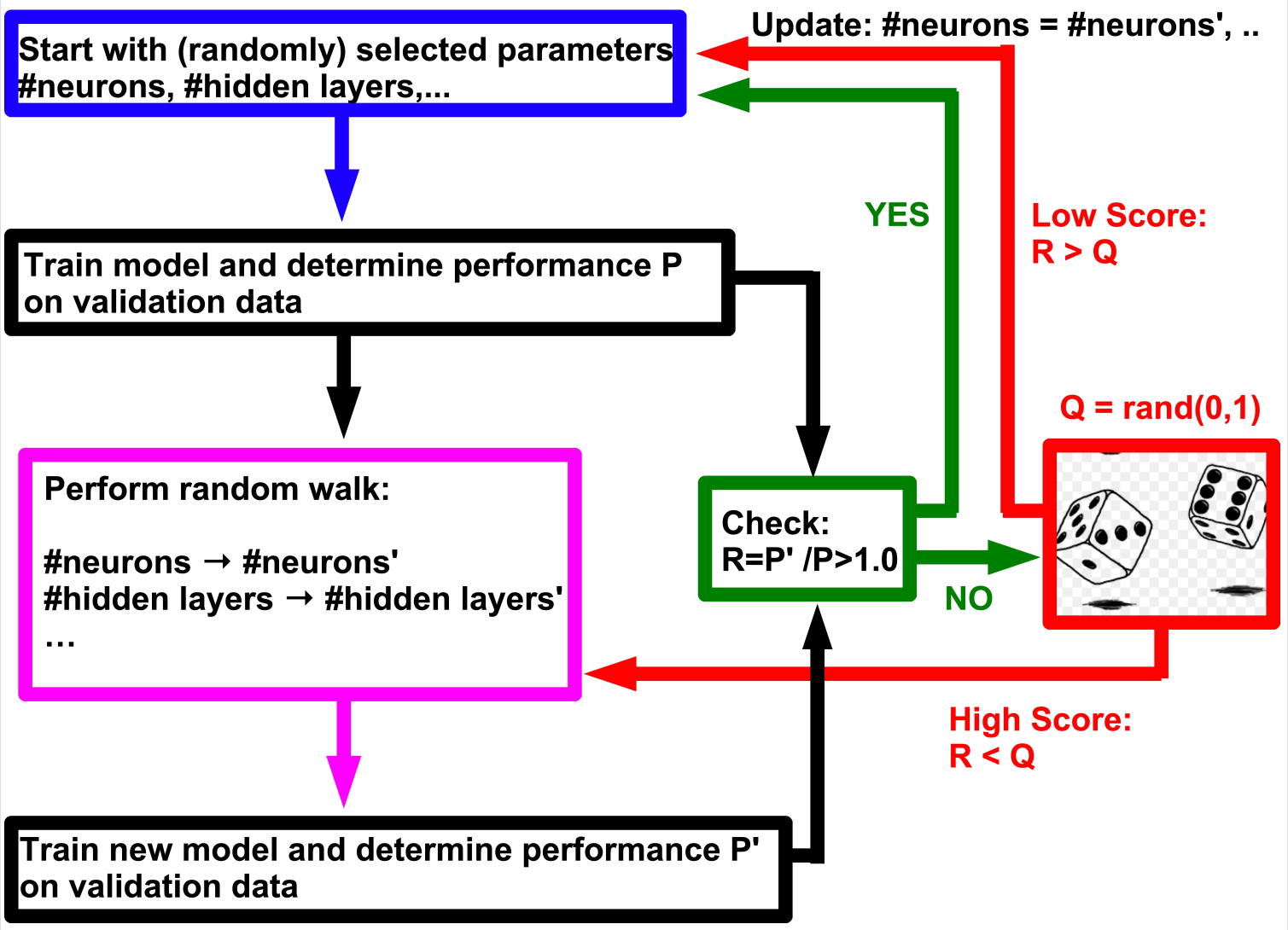
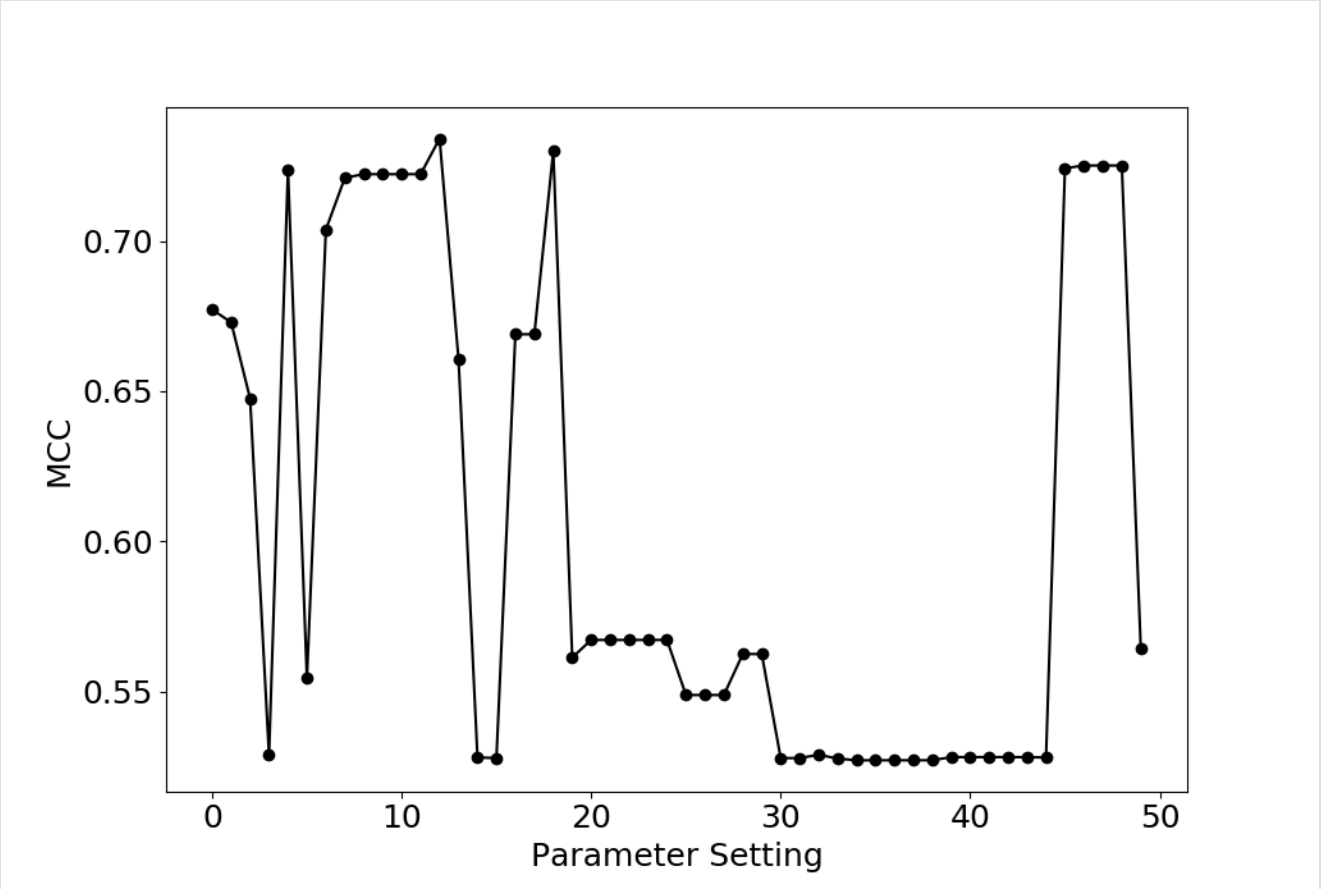


# Results Random Search



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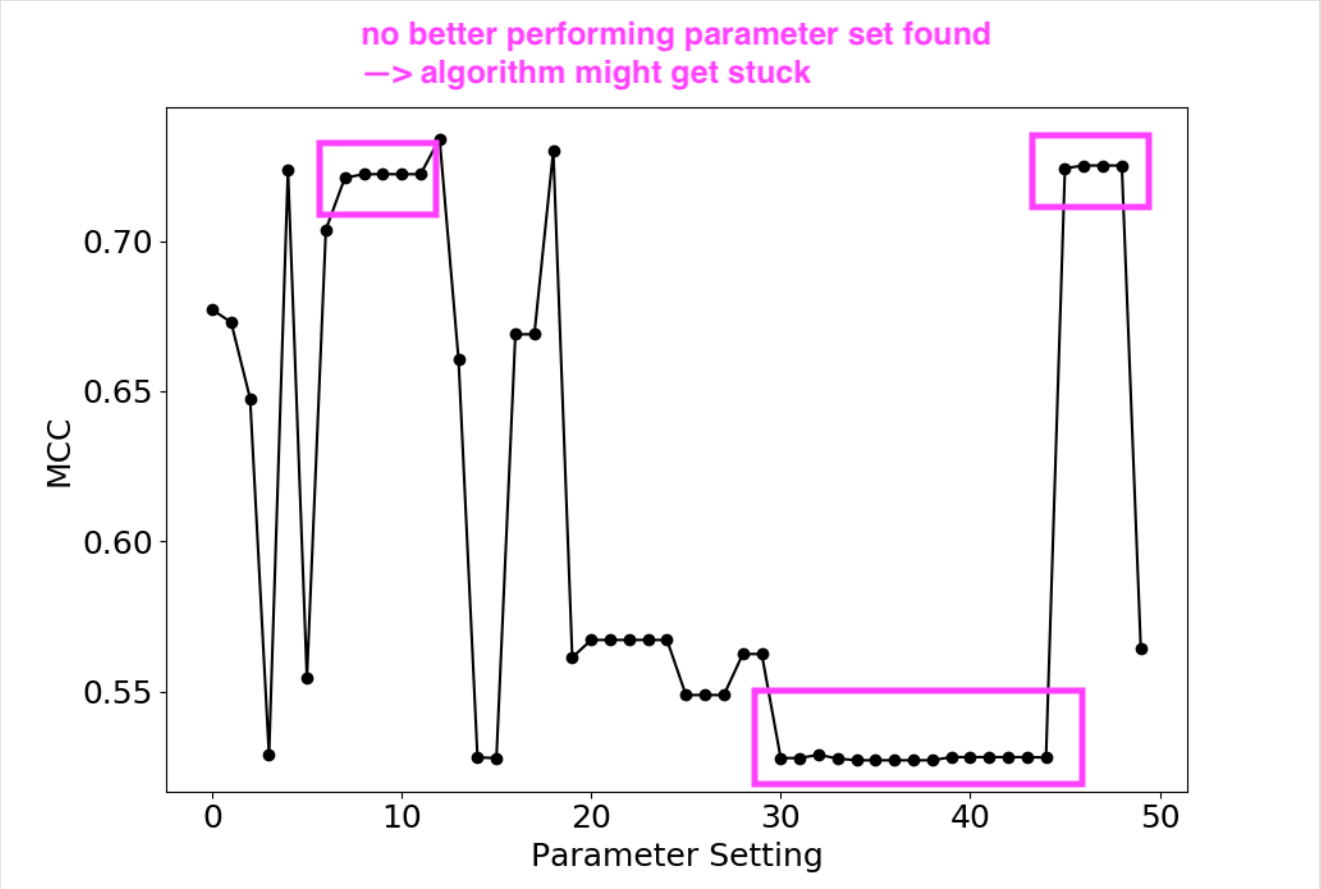

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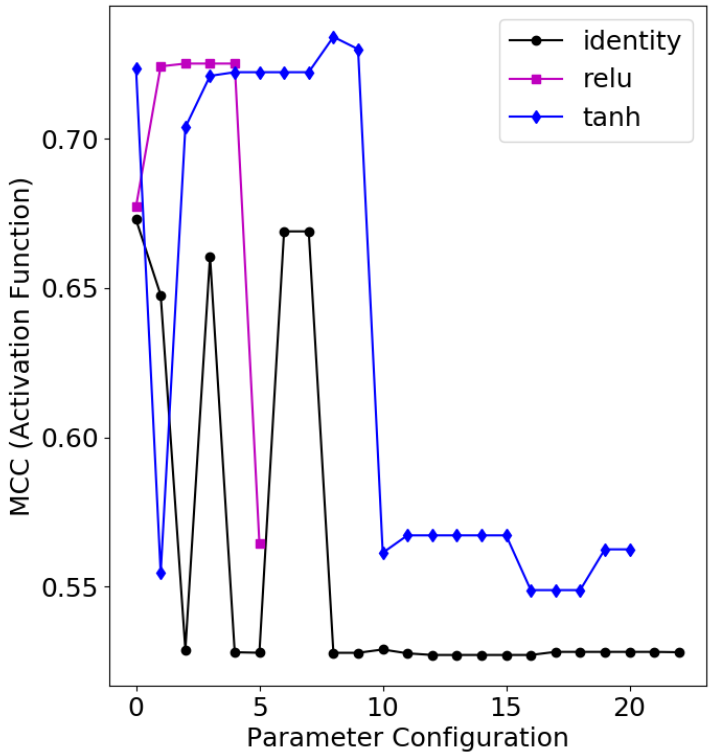


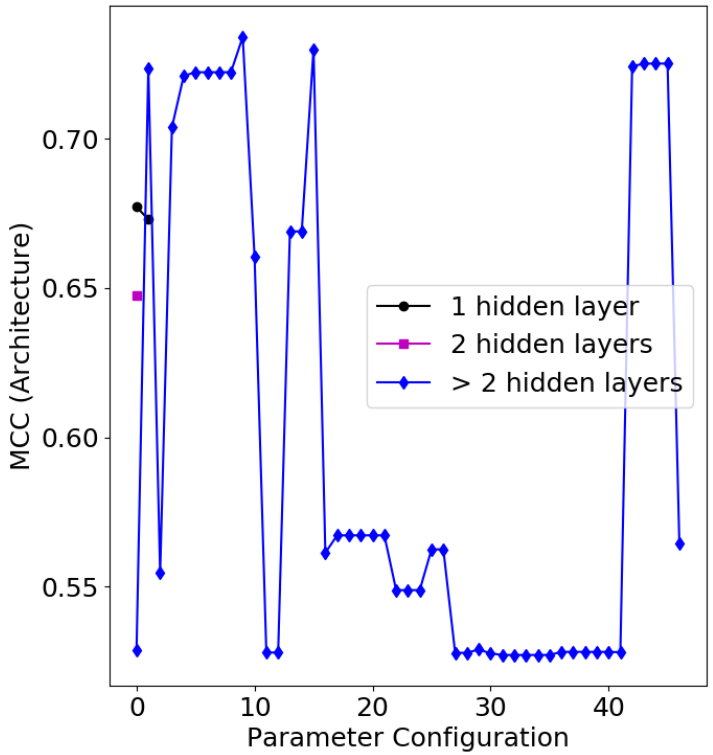

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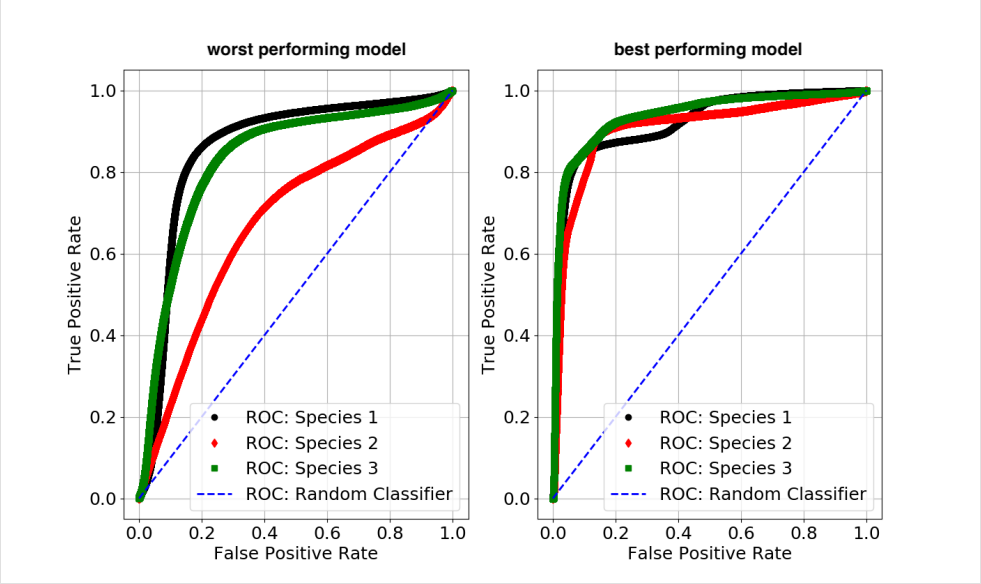

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- For example **Spearmint Bayesian Optimization**

# From Machine to Deep Learning: An Example

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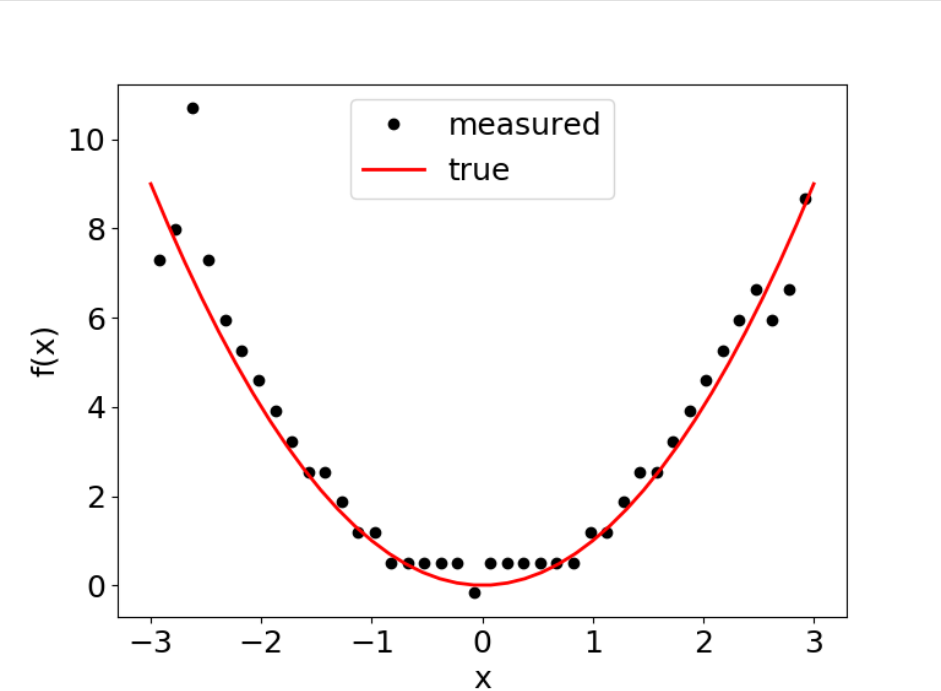

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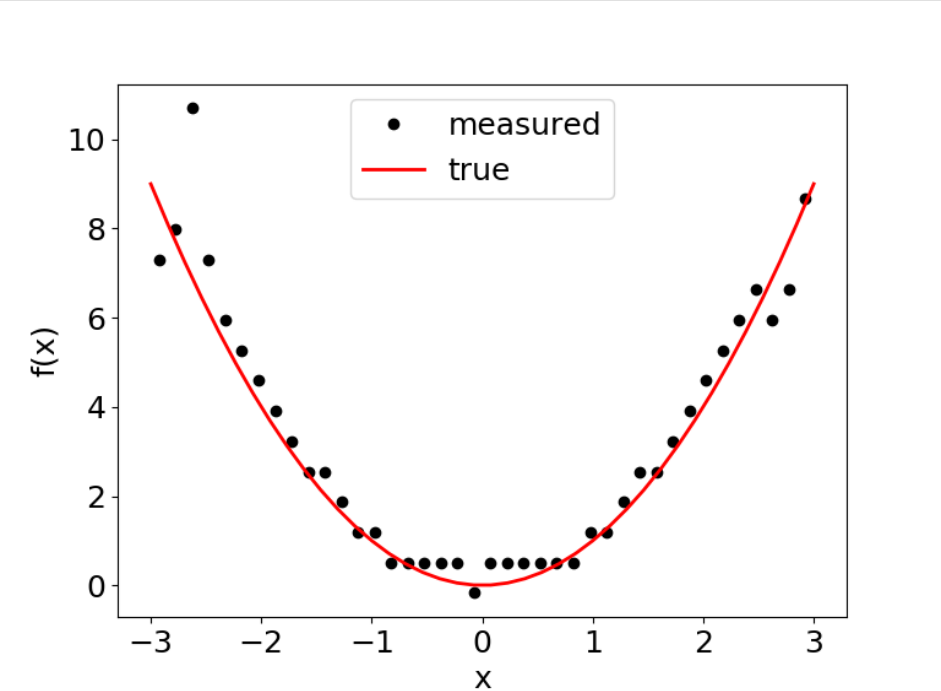


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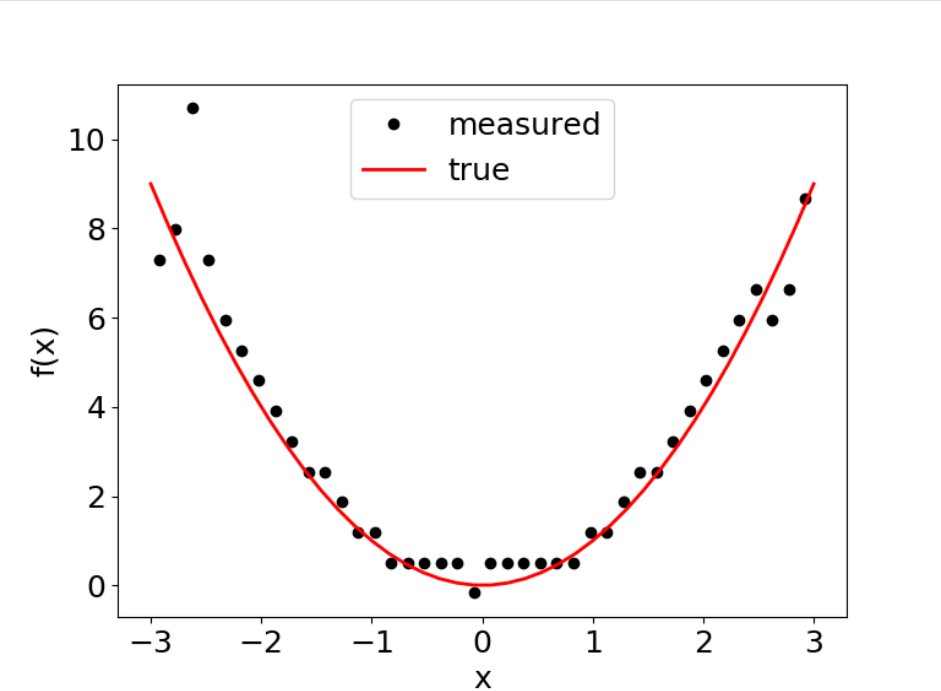


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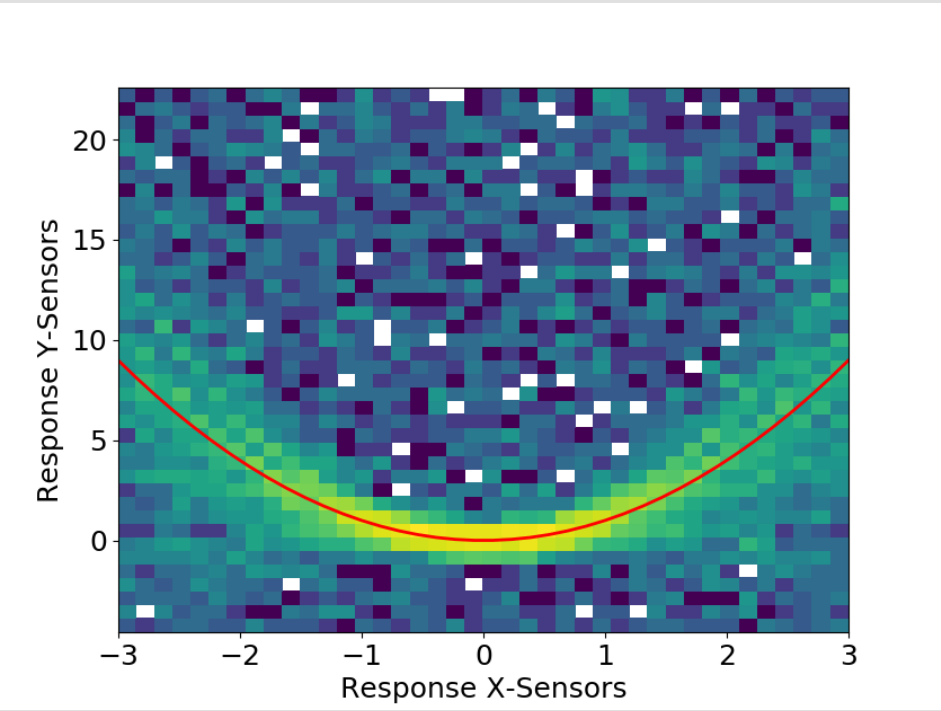

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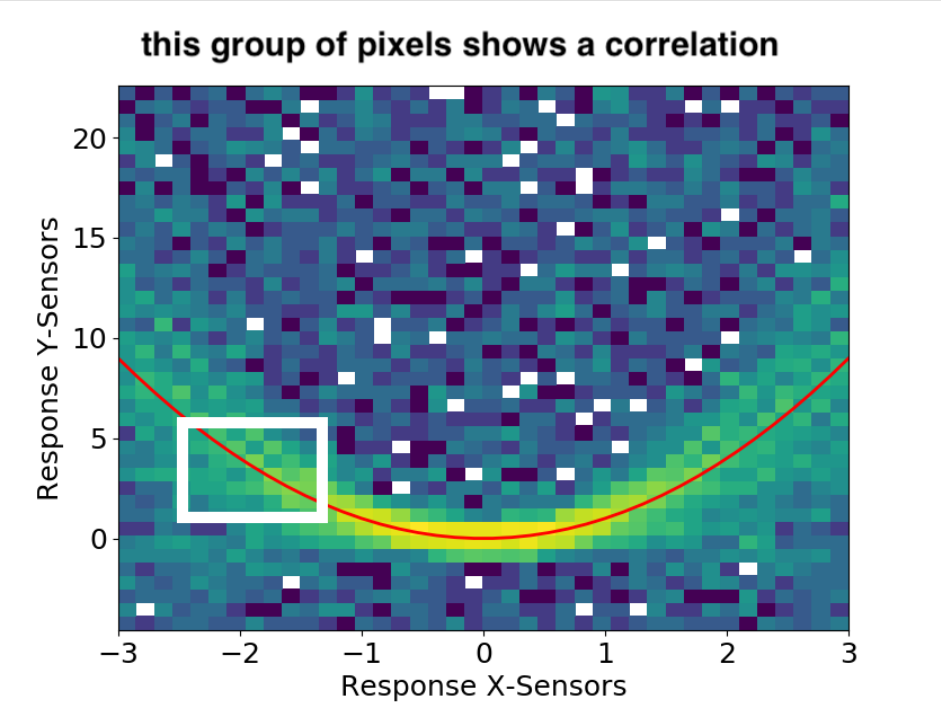

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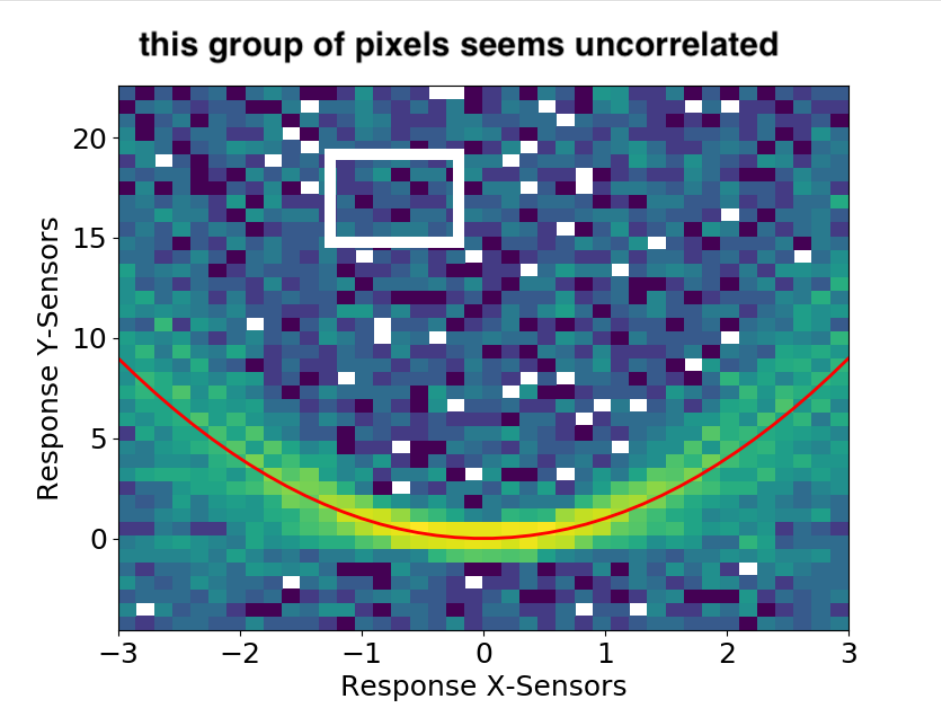

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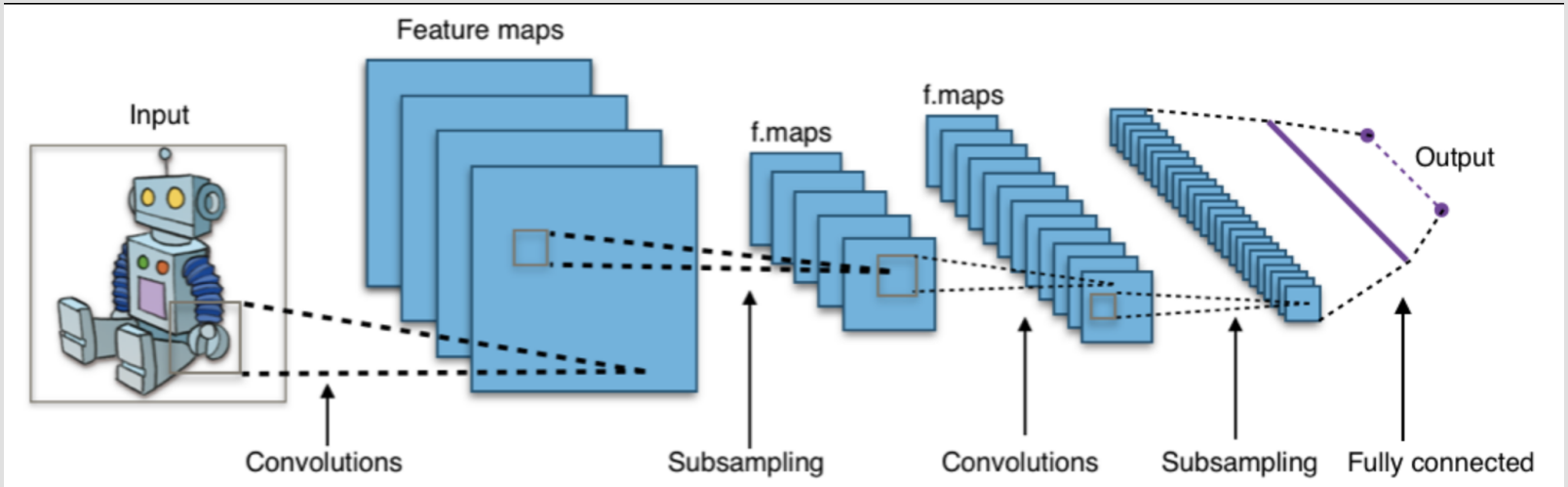


**Picture taken from** Aphex34 @ wikipedia

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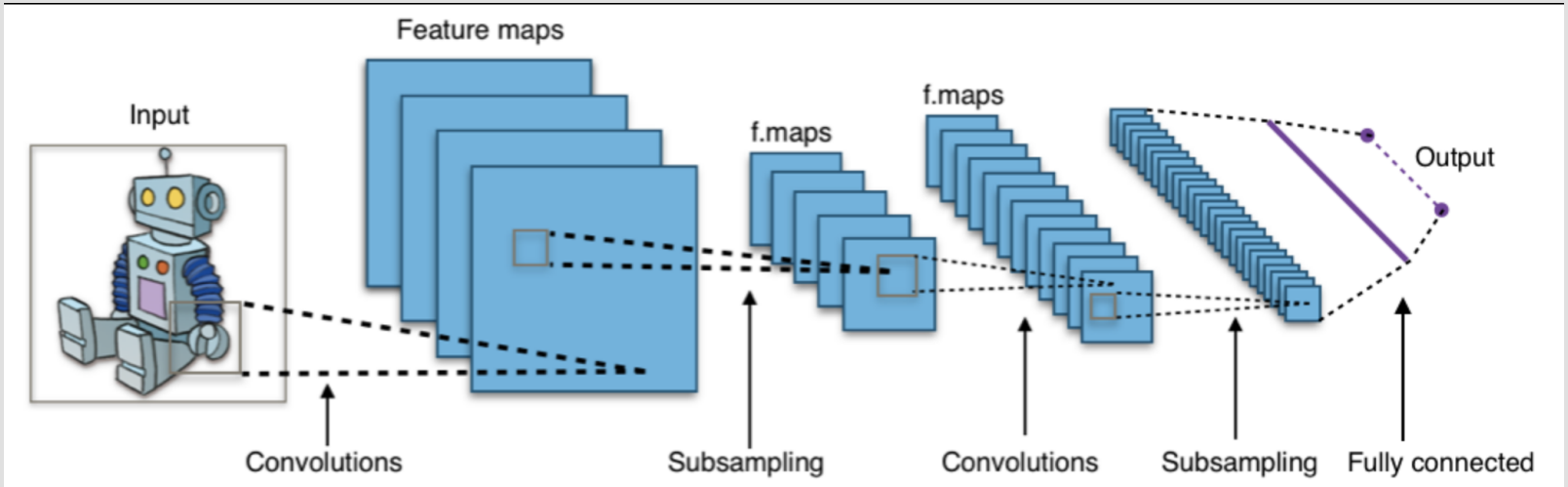


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- Many parameters ($\sim 1000\,\mathrm{k}$) to tune!

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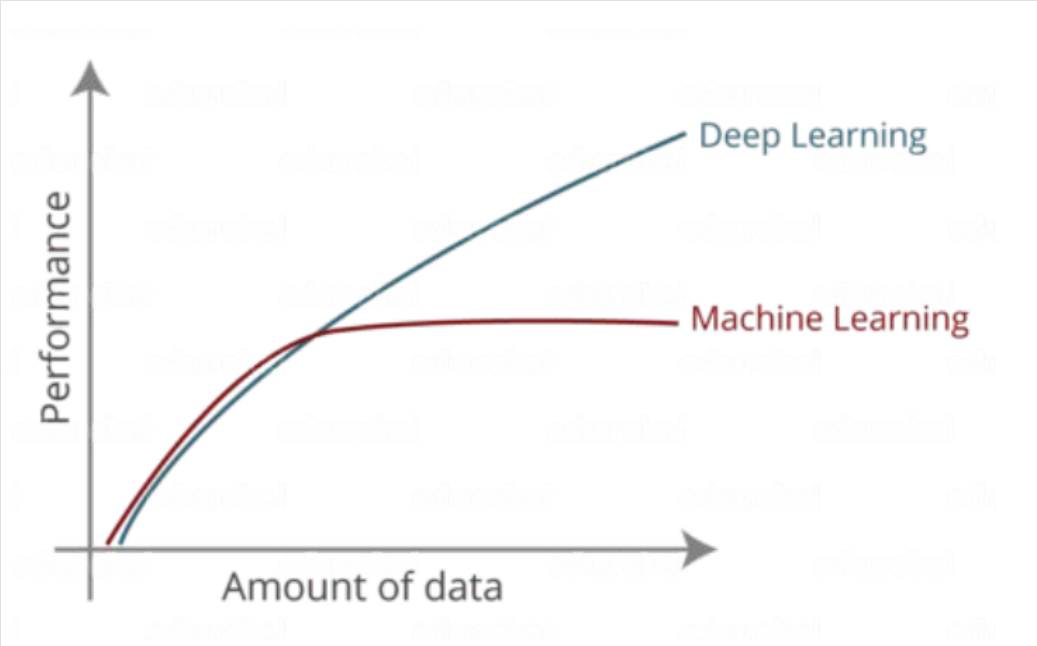


Picture taken from Mustafa Mustafas talk at the: deep learning for science school 2019

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- The following slides will show a simple example on how to setup a mlp in Tensorflow

# Setting up the Classification MLP in Tenserflow / Keras

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```
import tensorflow as tf

mlp_model = tf.keras.Sequential()
```

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```
#First hidden layer:
first_hidden_layer = tf.keras.layers.Dense(
    units=(5),
    input_shape=(3,), #---> we have three input variables
    #no need to define shape for following layers
    activation='tanh',
    kernel_initializer='glorot_normal', #--> Very important!
    bias_initializer='glorot_normal'
)

another_hidden_layer = tf.keras.layers.Dense(...)

final_layer = tf.keras.layers.Dense(
    units=(3), #---> We have three outputs
    activation='softmax', #---> Same function as used in scikit
    kernel_initializer='glorot_uniform',
    bias_initializer='zeros'
)
```

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```
mlp_model.add(first_hidden_layer)
mlp_model.add(another_hidden_layer)
mlp_model.add(final_layer)

#Define loss minimization technique
my_optimizer = tf.keras.optimizers.SGD(learning_rate=0.05)

#Compile the model:
mlp_model.compile(
    optimizer=my_optimizer,
    loss="categorical_crossentropy",
    metrics=['accuracy']
)

mlp_model.summary() #--> Print model setup
```

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```
Model: "sequential"
_________________________________________________________________
Layer (type)                 Output Shape              Param #
=================================================================
dense (Dense)                (None, 5)                 20
_________________________________________________________________
dense_3 (Dense)              (None, 3)                 18
=================================================================
Total params: 38
Trainable params: 38
Non-trainable params: 0
```

# Massaging the Data for the Model

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```
def get_label_vec(label):
    vec = [0,0,0]
    vec[int(label)] = 1 #--> label 1 = (0,1,0), label 2 = (0,01),..

    return vec

data_df['label_vec'] = data_df['label'].apply(
    lambda x: get_label_vec(x)
)
```

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| | var1 | var2 | var3 | label | label_vec |
|---|---|---|---|---|---|
| 0 | 2.140464 | 0.871710 | 1.634352 | 2.0 | [0, 0, 1] |
| 1 | 1.788192 | 1.992385 | 2.423125 | 1.0 | [0, 1, 0] |
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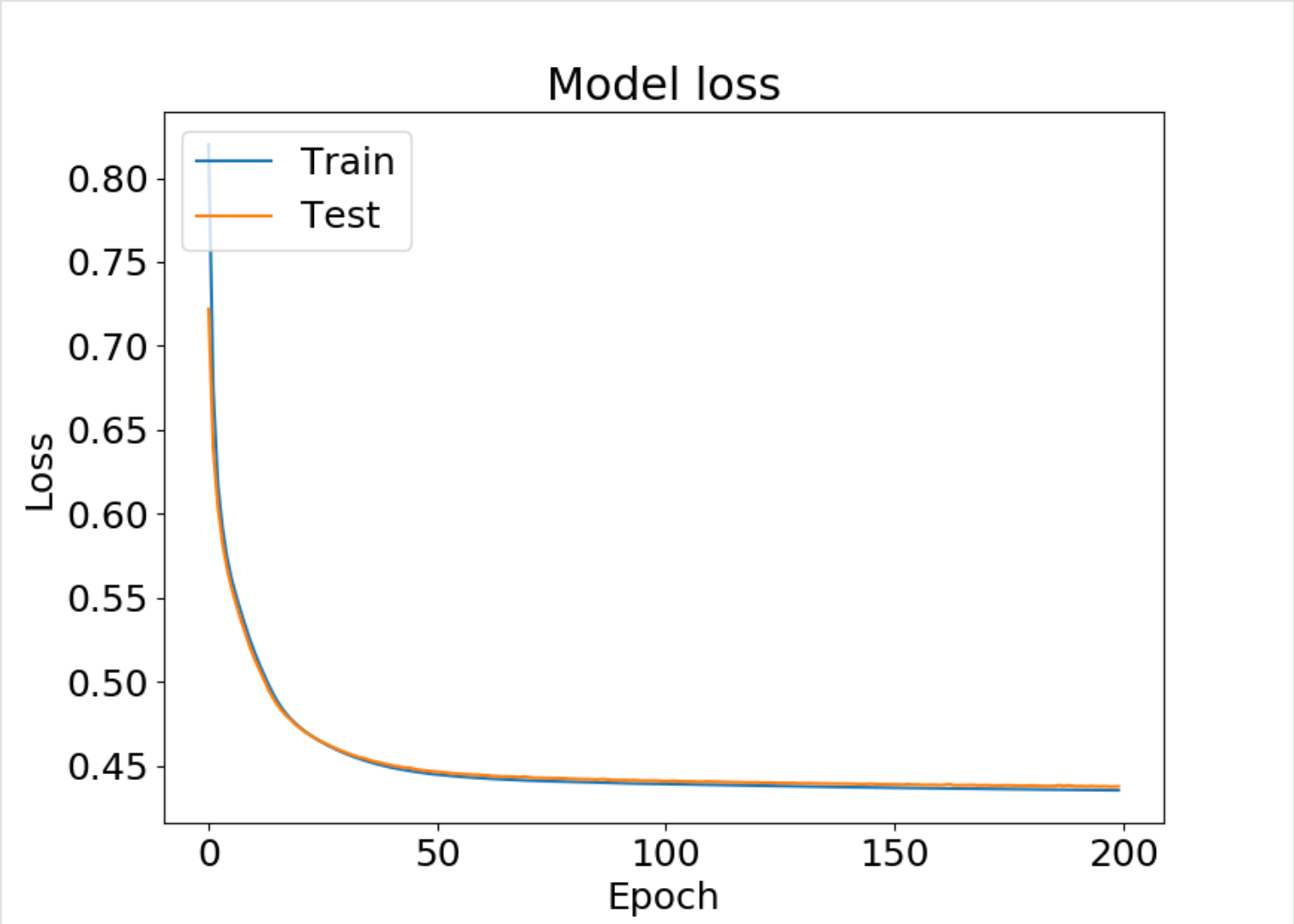
```
#Train model:
history = mlp_model.fit(
      X, #---> The three features
      Y, #---> The label vectors
      epochs=100, #--> number of epochs
      batch_size=200,
      validation_split=0.25
 )

#history summarizes the training history:
plt.plot(history.history['loss'])
plt.plot(history.history['val_loss'])
plt.title('Model loss')
plt.ylabel('Loss')
plt.xlabel('Epoch')
plt.legend(['Train', 'Test'], loc='upper left')

plt.show()
```

# Training the Model

- Like in scikit, call the fit-function
- Check the training curve



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```
def get_predicted_label(x):
    max_val = max(x) #---> Get the maximum output
    max_i = x.index(max_val) #--> Get the node index
    #which corresponds to the label

    return max_i

data_df['predicted_label'] = ...
```

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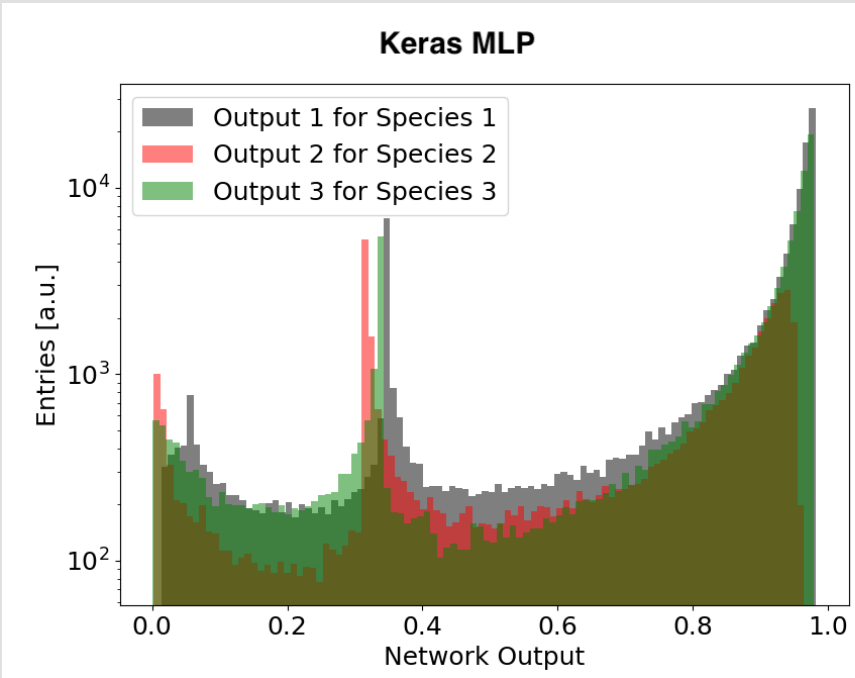


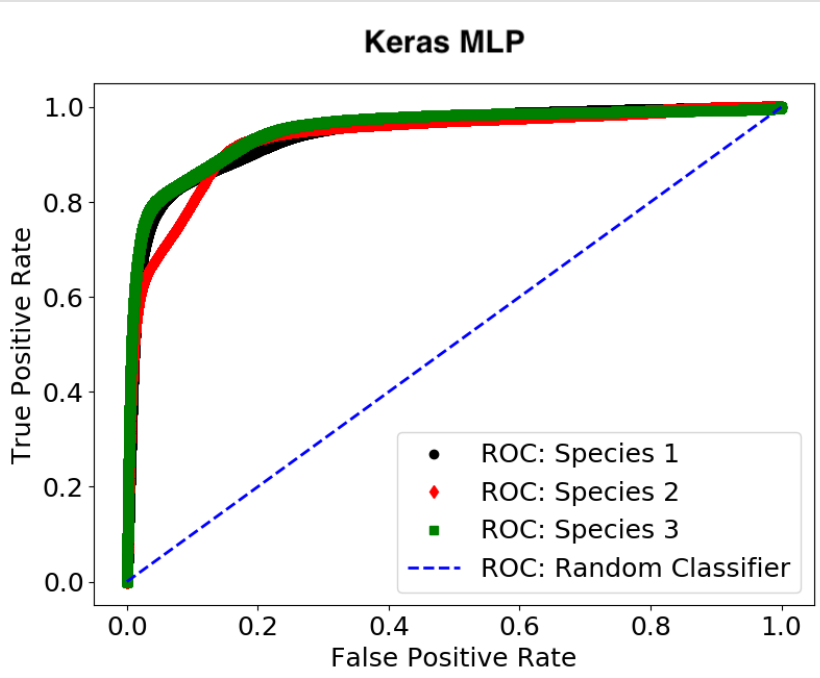

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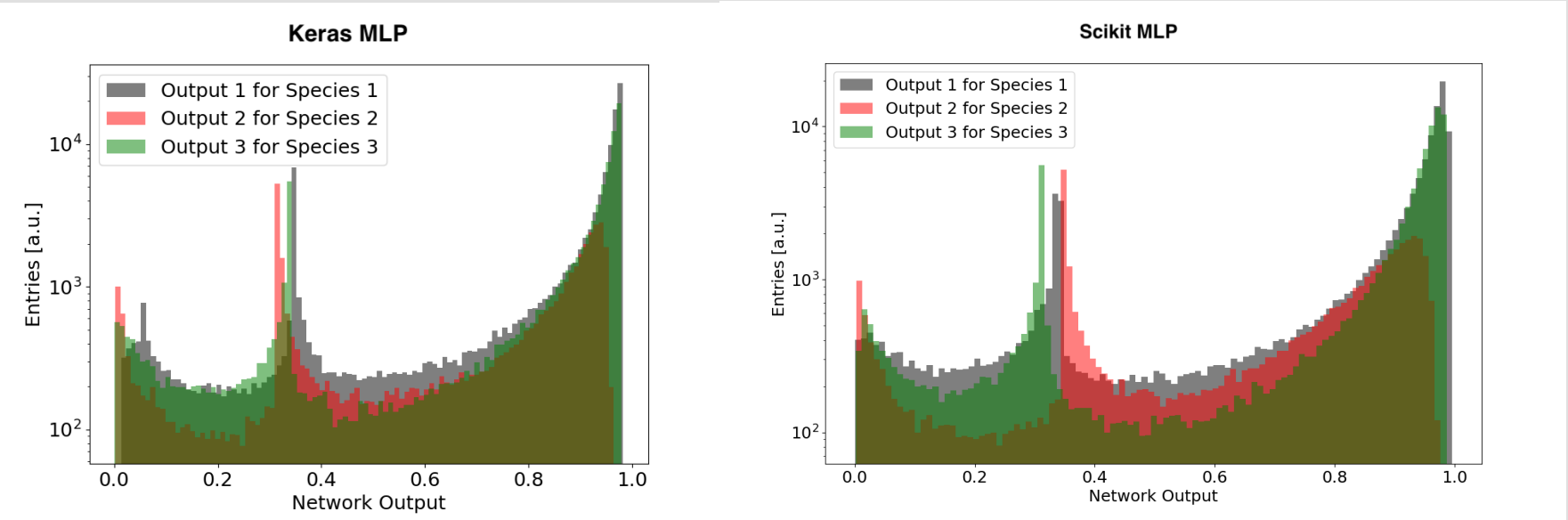

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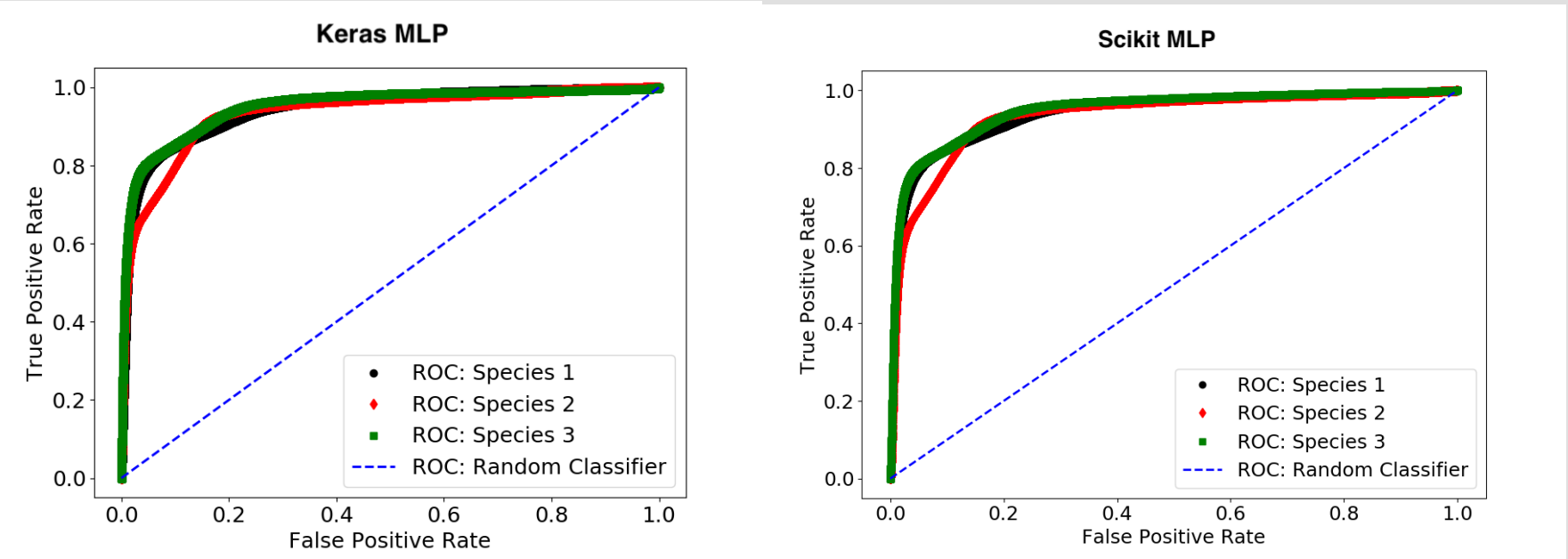

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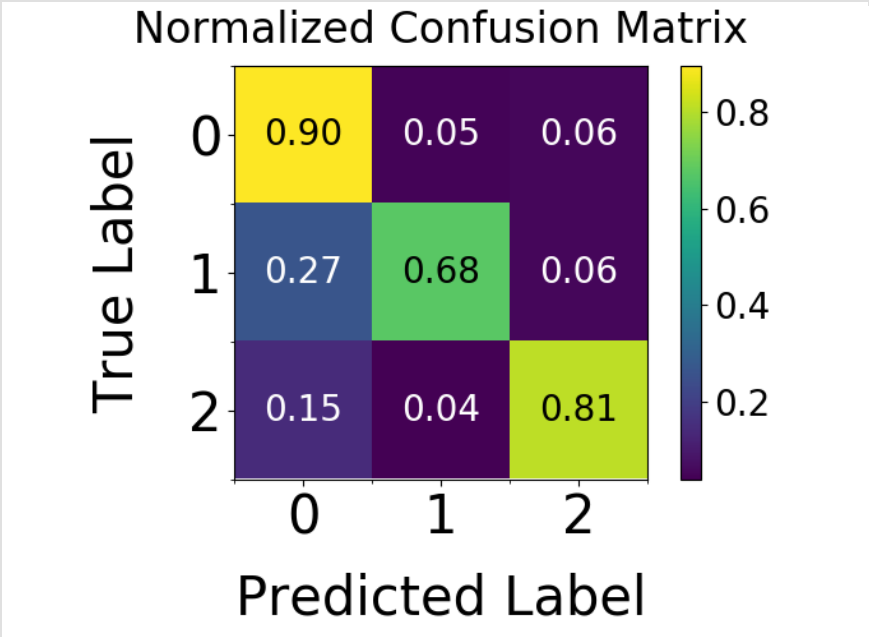


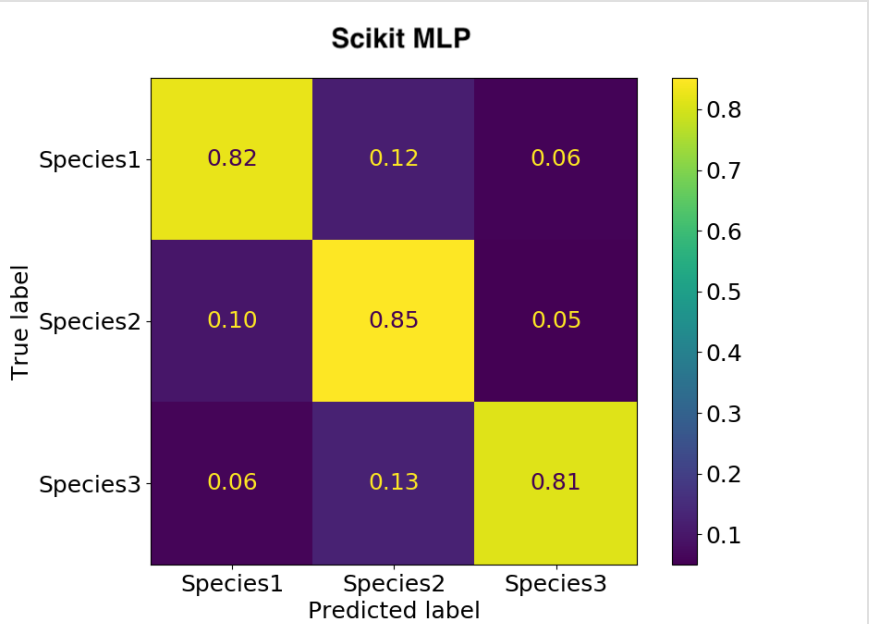

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- It is sometimes worth to compare different frameworks on the same problem $\rightarrow$ Check for consistency

# A few Words on Tensors

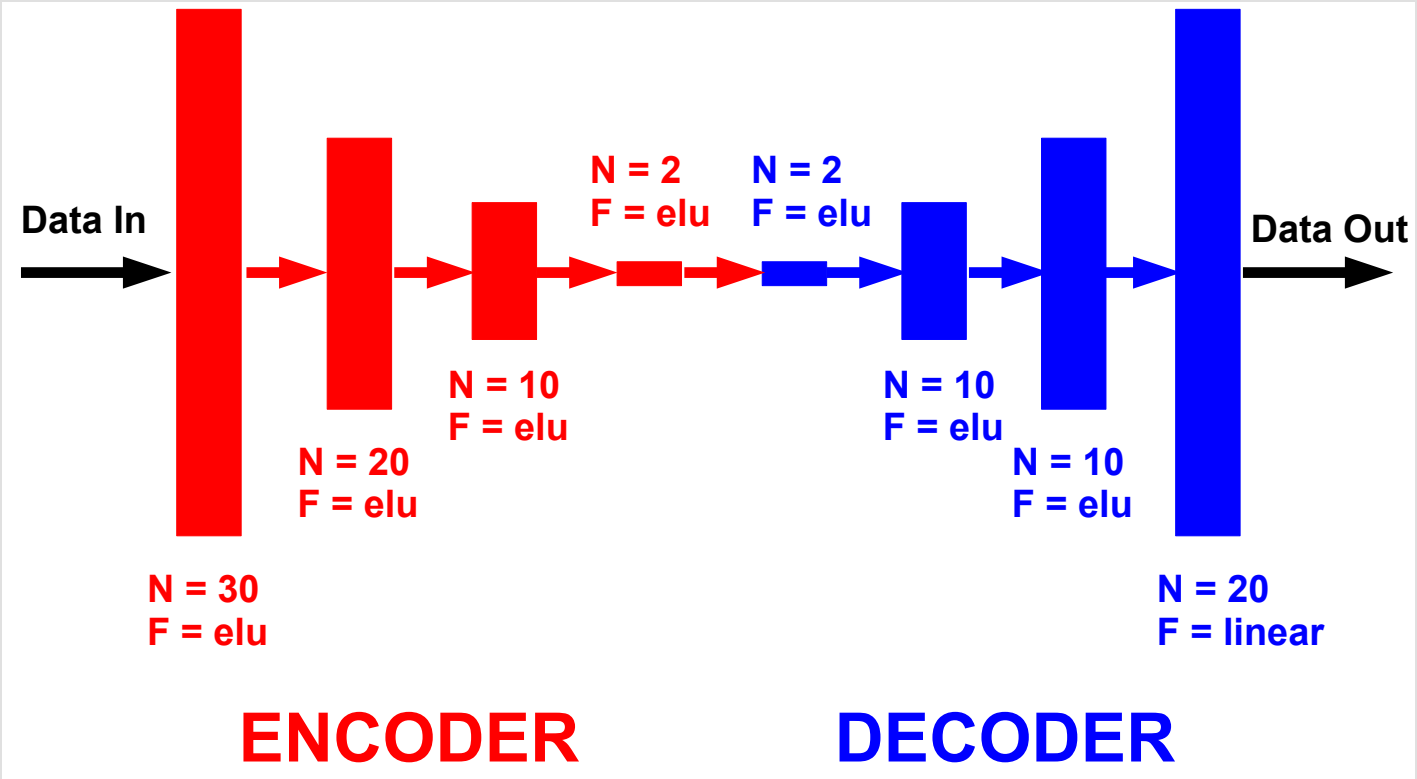
- As the name suggests, Tensorflow uses tensors which are multidimensional objects with rank and shape
- The following examples are taken from the **Tensorflow web-page**

| Rank | Shape | Dimension number | Example | |
|---|---|---|---|---|
| 0 | [] | 0-D | A 0-D tensor. A scalar. | **a single number** |
| 1 | [D0] | 1-D | A 1-D tensor with shape [5]. | **a 5-dim vector** |
| 2 | [D0, D1] | 2-D | A 2-D tensor with shape [3, 4]. | **a 3x4 matrix** |
| 3 | [D0, D1, D2] | 3-D | A 3-D tensor with shape [1, 4, 3]. | **a cube** |
| n | [D0, D1, ... Dn-1] | n-D | A tensor with shape [D0, D1, ... Dn-1]. | **I am lost...** |

- This allows for a high flexibility regarding data input and mathematical operations (i.e. weight multiplication in a deep dense neural net)
- BUT: You have to ensure that the shape of your data and your input layers match!!!

# Deep Learning in GlueX Physics

- Use autoencoder for electron / pion identification
- Features: $p$, $\theta$, $dE/dx(CDC)$, $E(BCAL)$ and $E(FCAL)$
- Number of input nodes = 5 = Number of output nodes
- Use tied weights during training $\rightarrow$ Reduce number of trainable parameters




**N: Number of neurons in dense hidden layer**
**F: Activation function in dense hidden layer**

# Machine / Deep Learning vs. Fitting a Function

| | ML / DL | Fit Function (e.g Gauss, pol(N),...) |
|---|---|---|
| Parameters | weights, nodes,... | mean, width, $p_i \cdot x^i$, ... |
| Hyper Parameters | learning rate, architecture, learning epochs, tolerance,... | order of pol., include tails, fit iterations, tolerance,... |
| Optimizer | Adam, SGD, L-BFGS,... | $\chi^2$, Log-Likelihood |
| Data Sets | training, validation,.. bootstrapping | same here |
| Performance Evaluation | Mean squared error,... | $\chi^2$/ndf,... |
| Basic question | Which model? | Which fit function? |
| ... | ... | ... |

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  - Do not try to fine tune a random forest classifier on a complex data set (e.g. $\sim 100$ different correlated variables), if you can not achieve a reasonable performance

# References and Further Reading

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- I hope you had fun!