Introduction to Machine Learning: Part III

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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... 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

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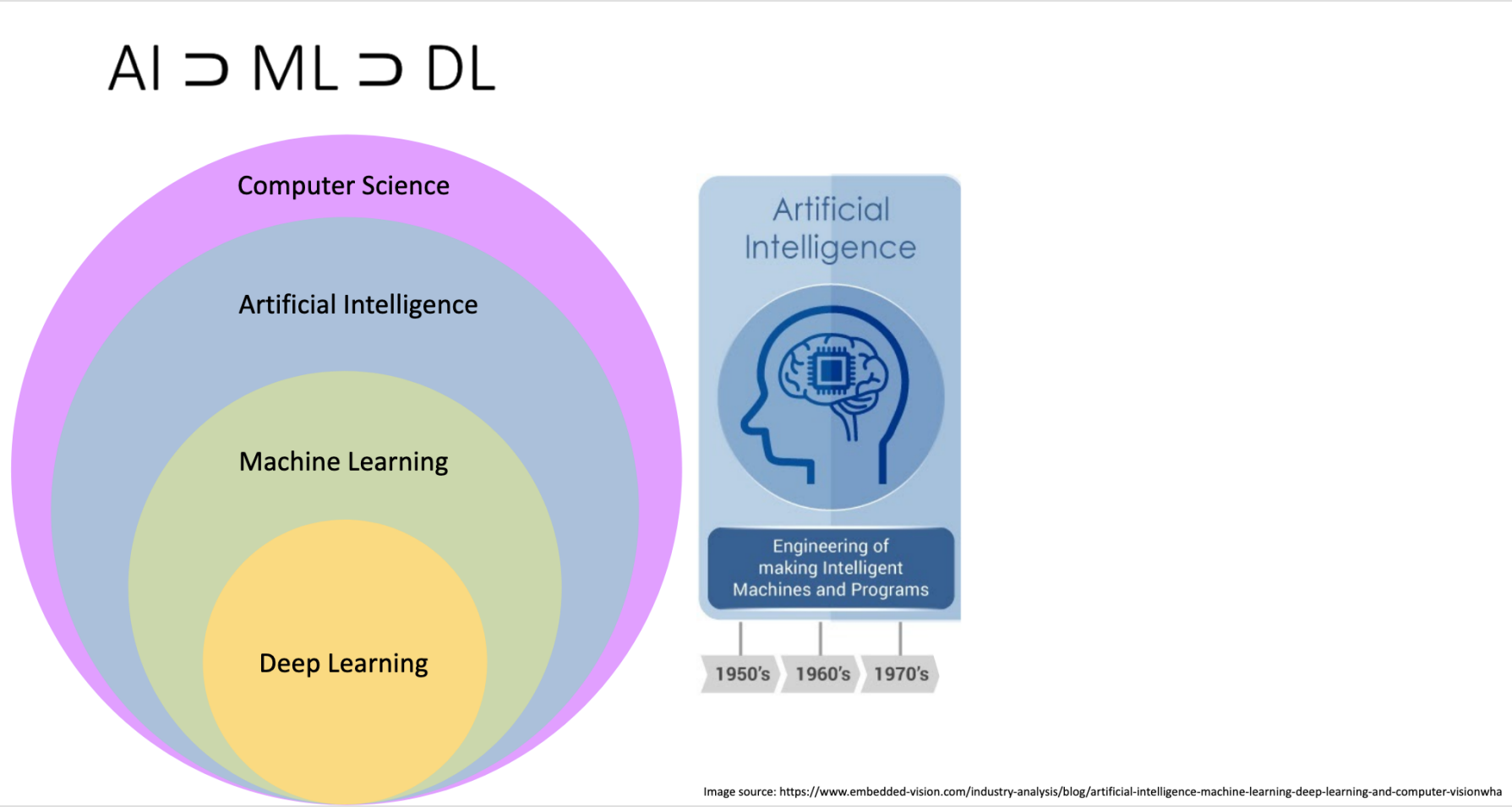
- Homework (most likely posted on Thursday) aims to perform a simple analysis and getting familiar with machine learning
- Helpful literature:
  - The **scikit-learn** documentation
  - Talks from the **deep learning for science school 2019**[3]
  - "Hands-On Machine Learning with Scikit-Learn, Keras & 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



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

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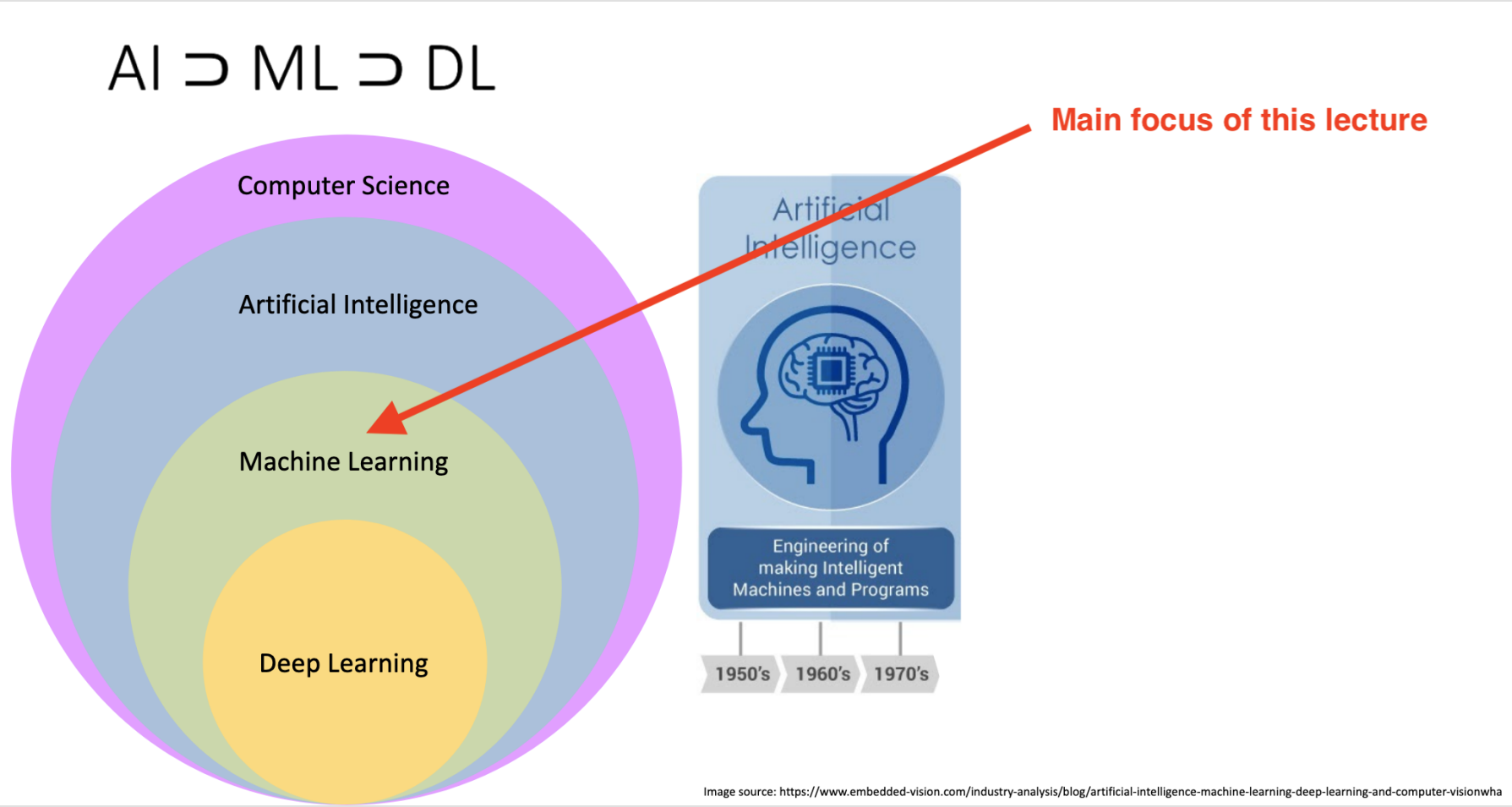

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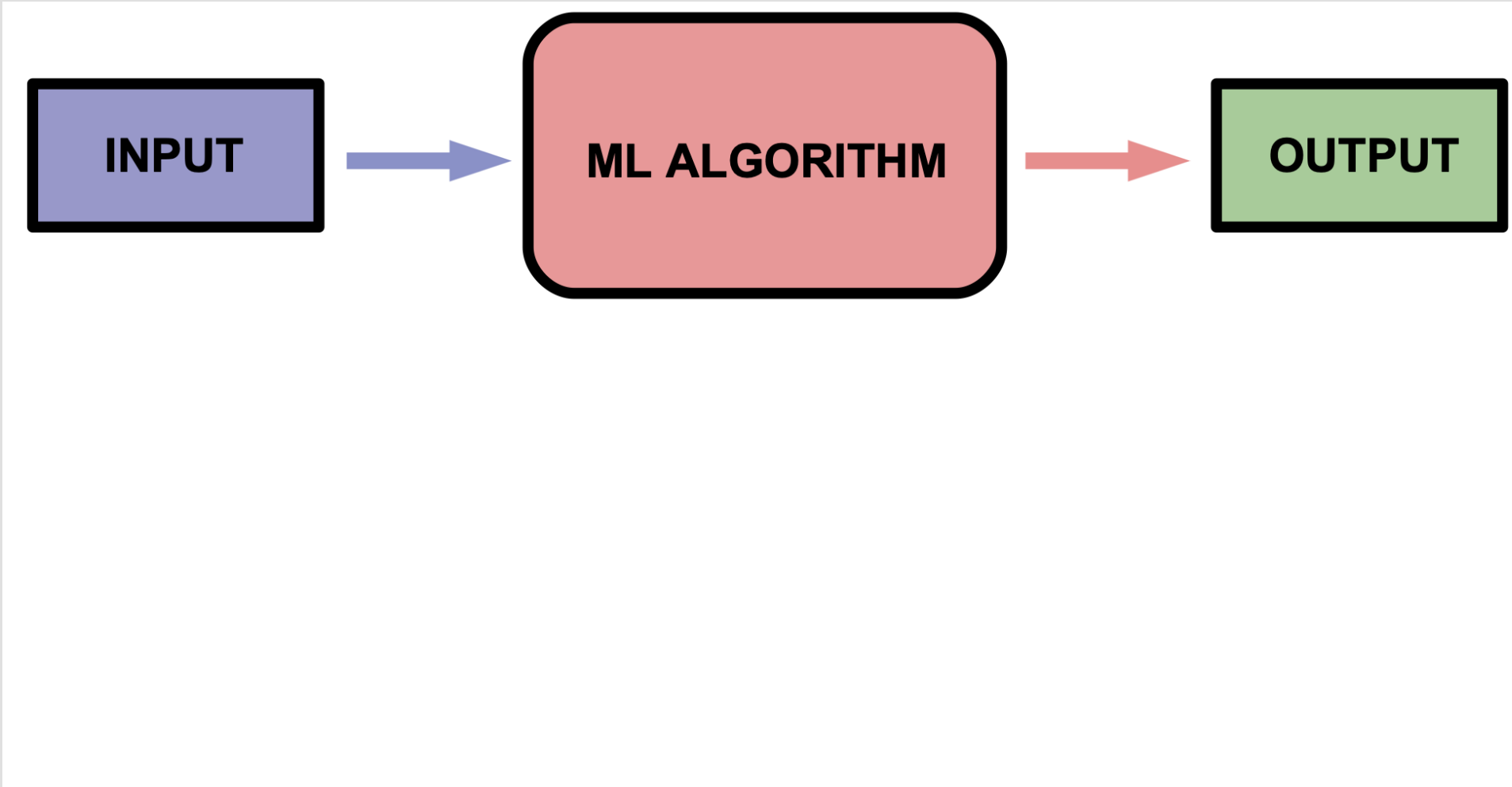

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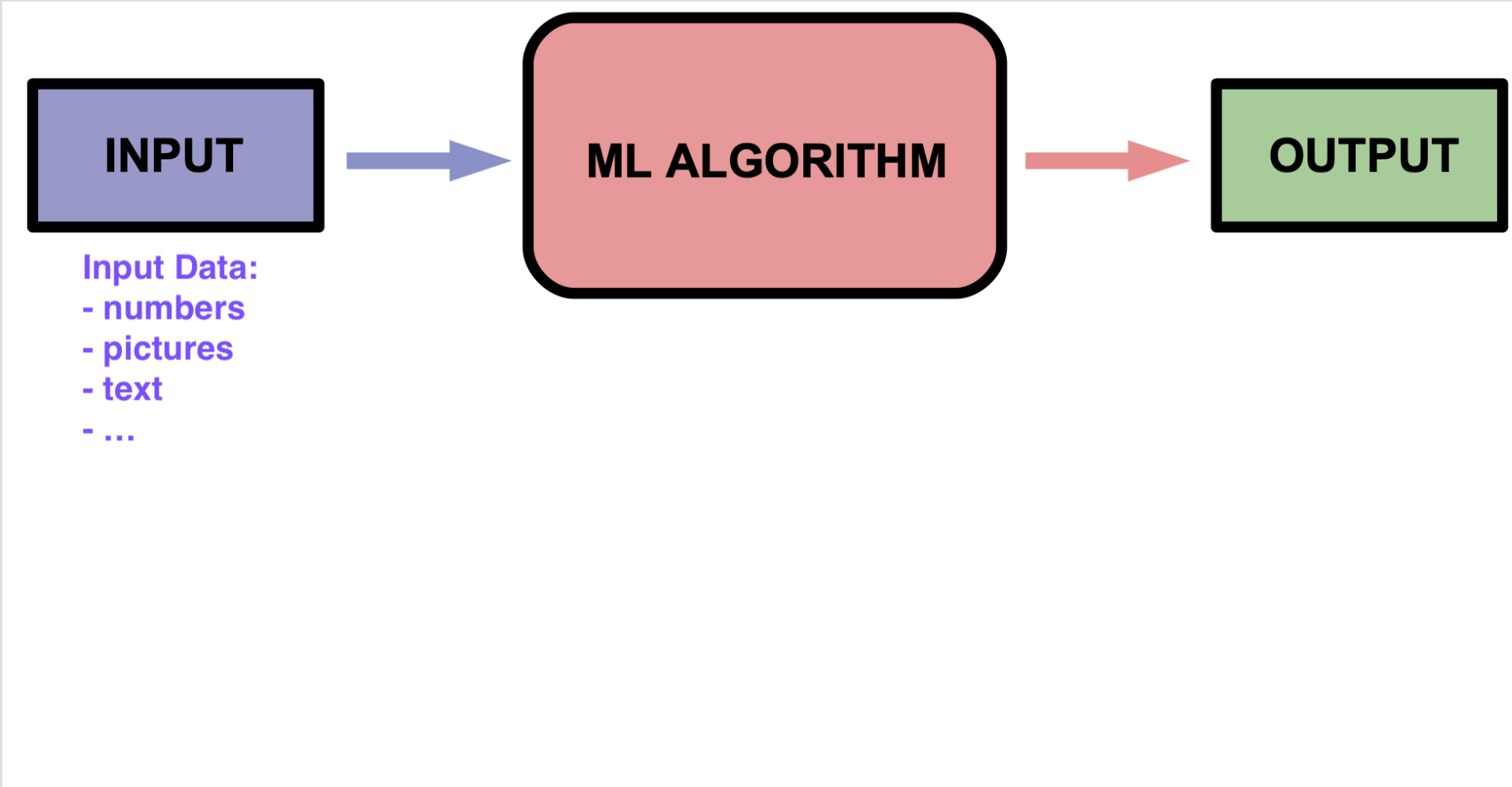

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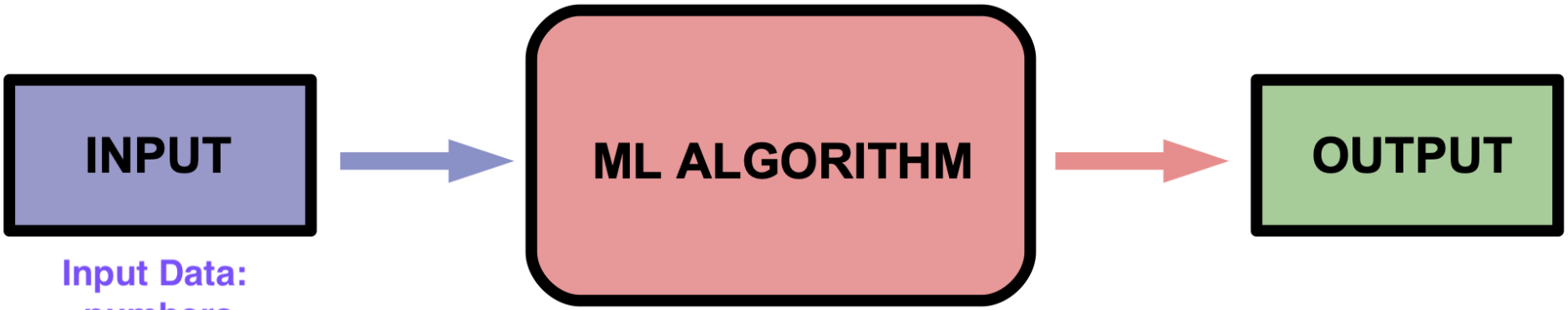

Input Data:
- numbers
- pictures
- text
- ...

Introduced in part I: DataFrames —> handle and manipulate data

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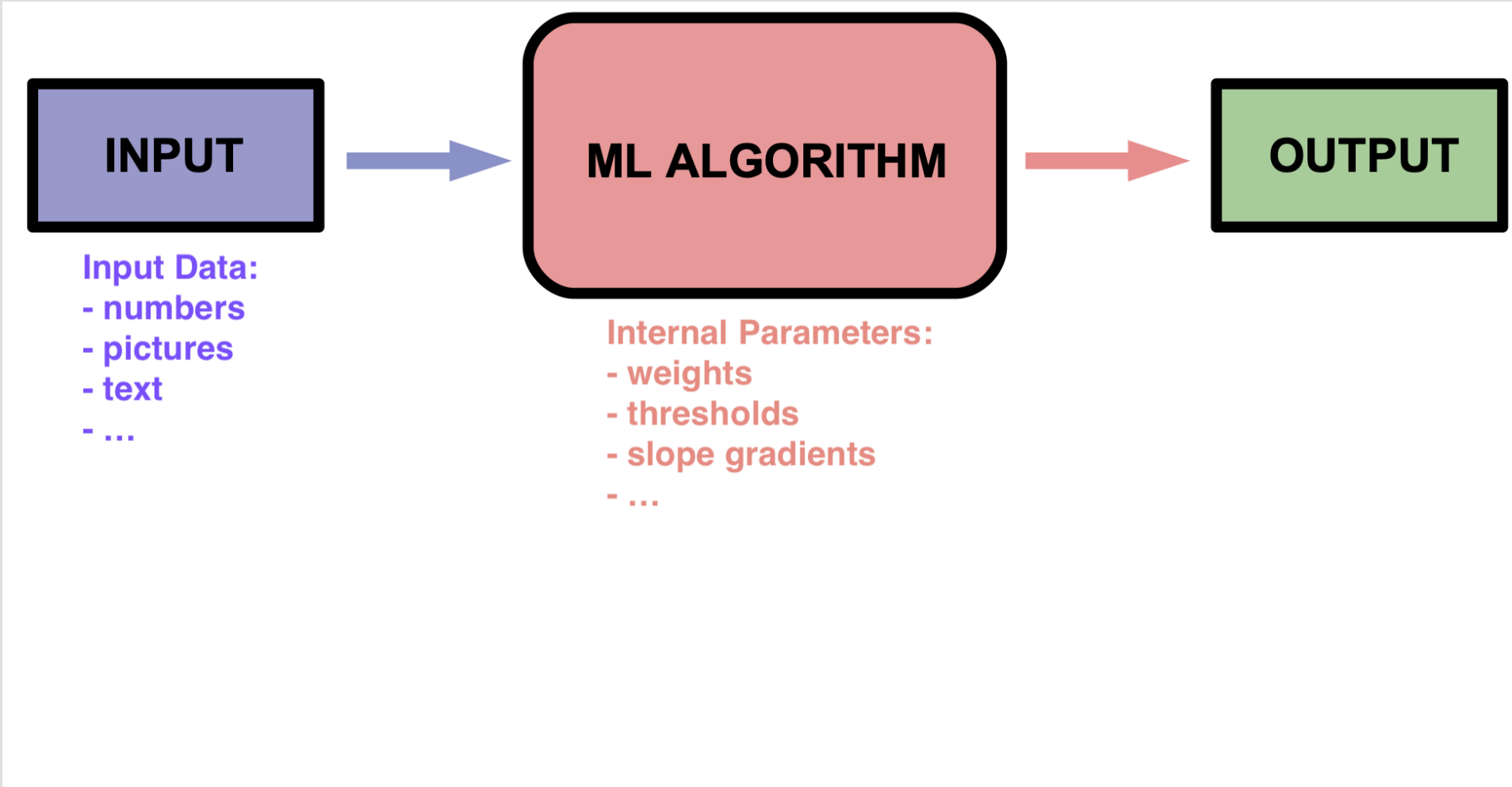

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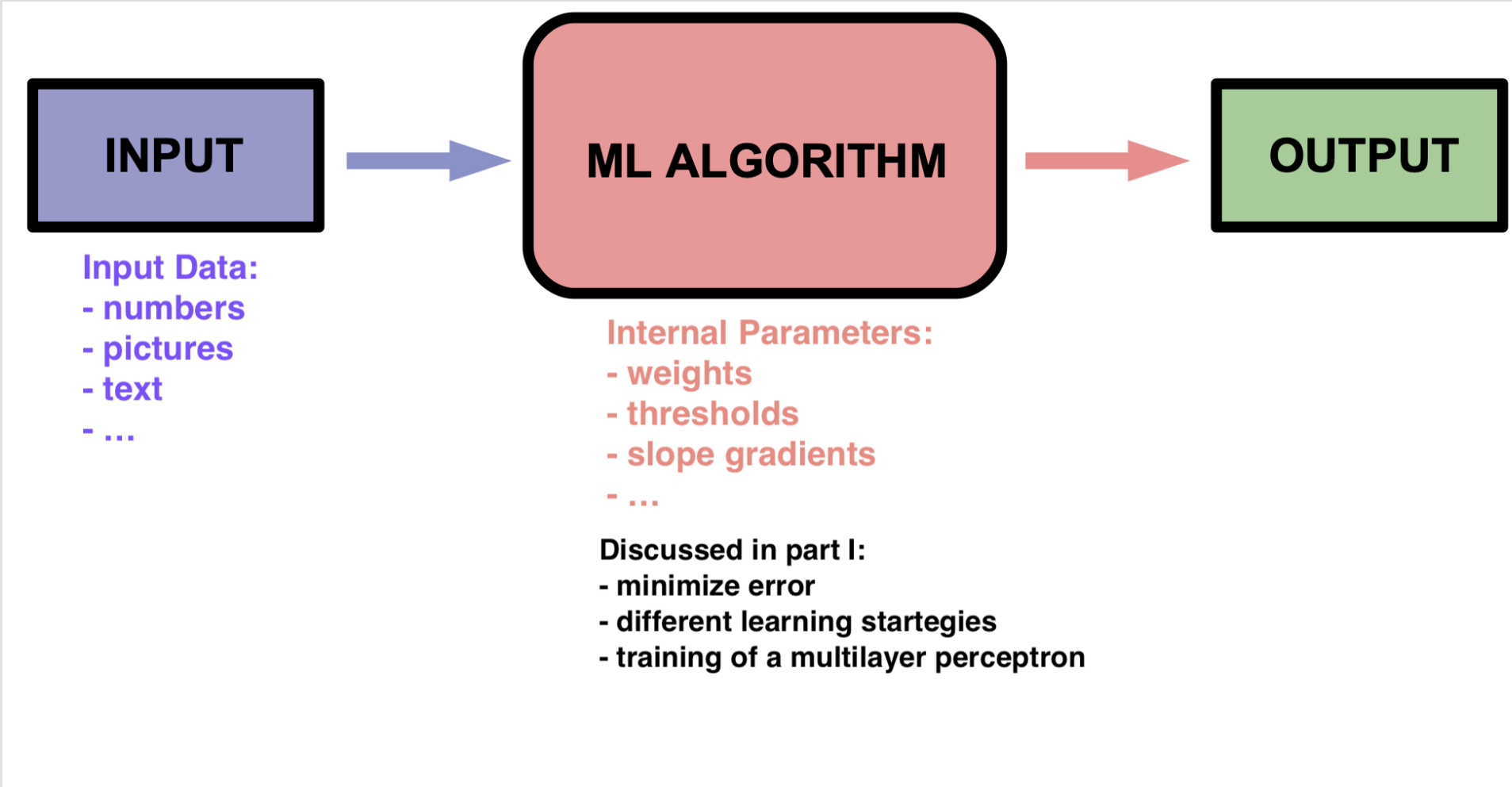

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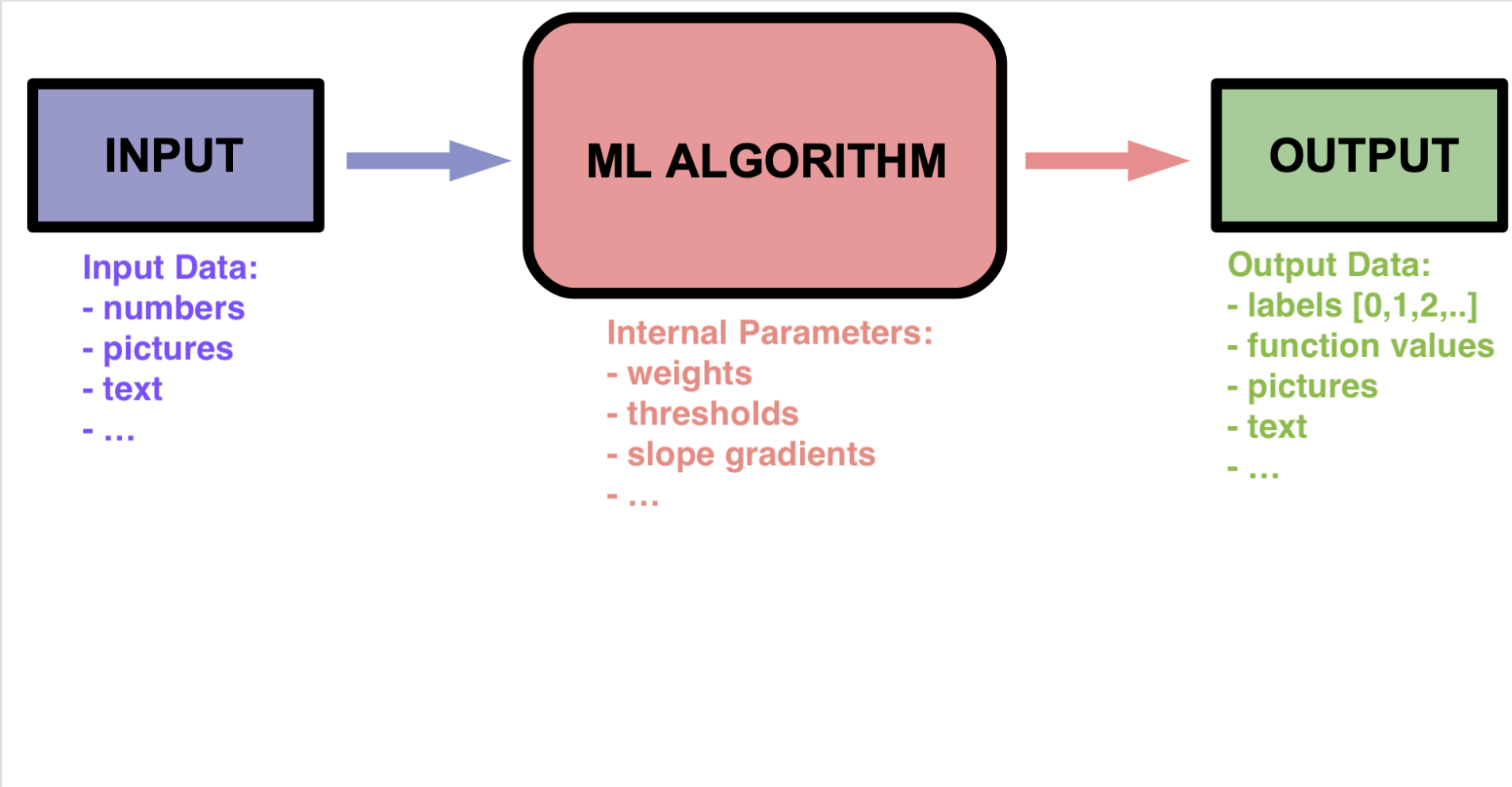

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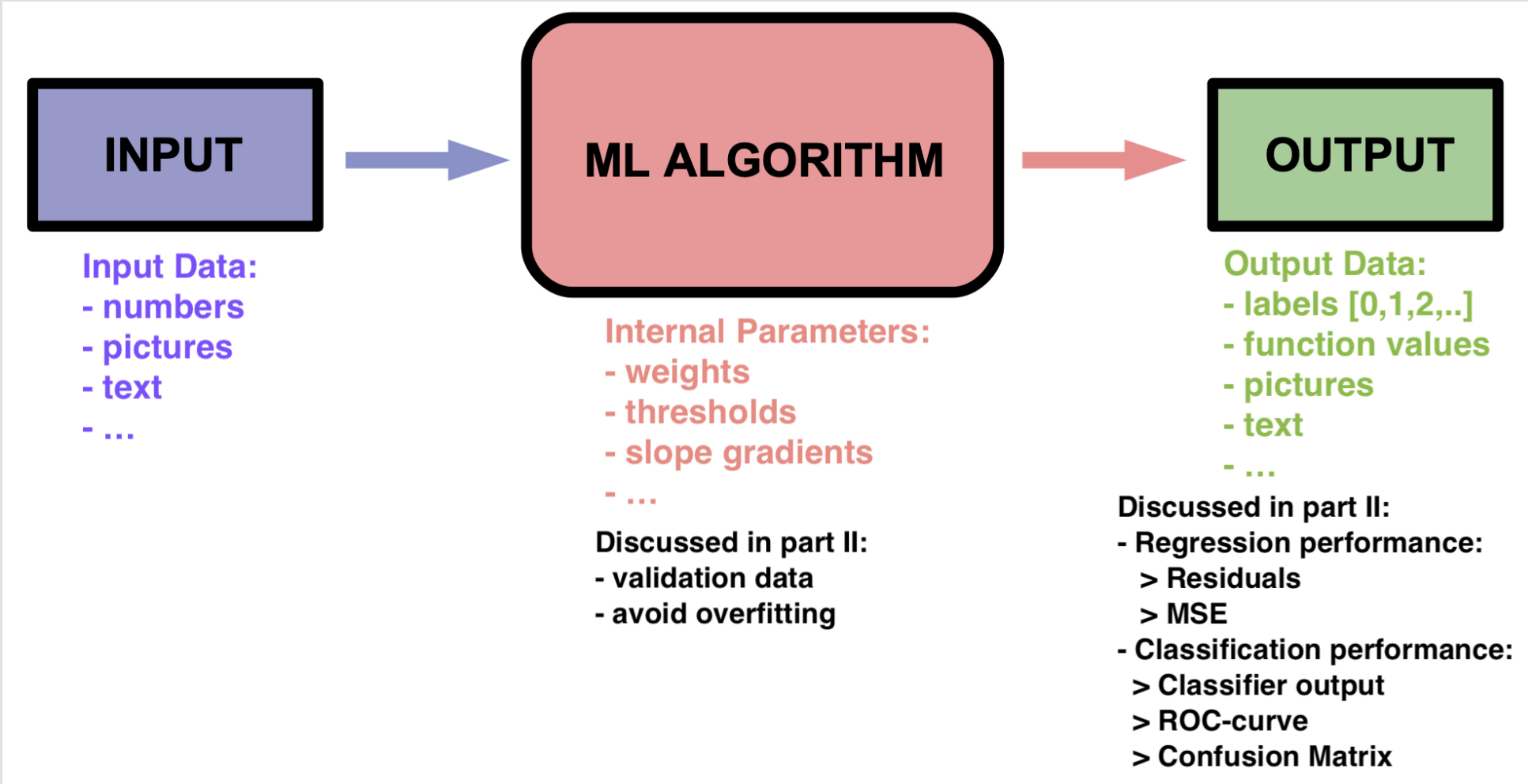

Classification with Machine Learning II

- In Part II: Discussed in detail a classification analysis, using a MLP
- But sometimes a MLP is not the best choice for the underlying problem / data
- Introduce X more classification algorithms which are an alternative to MLPs

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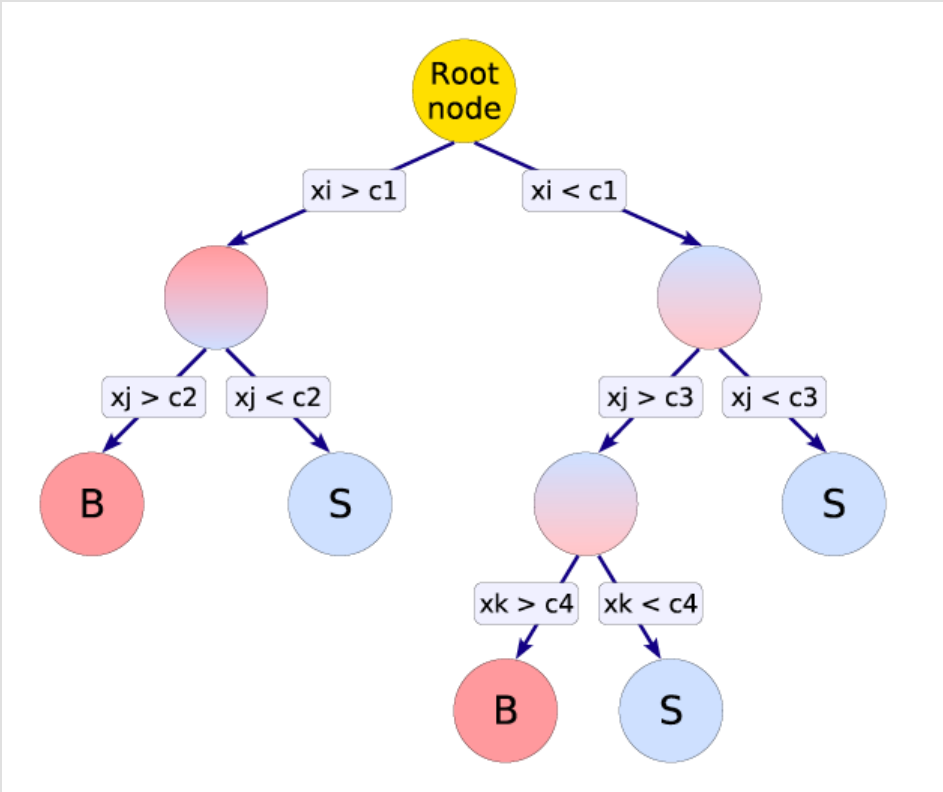

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- The detailed implementation of a random forest will not be discussed here $\leftrightarrow$ Already done in the homework

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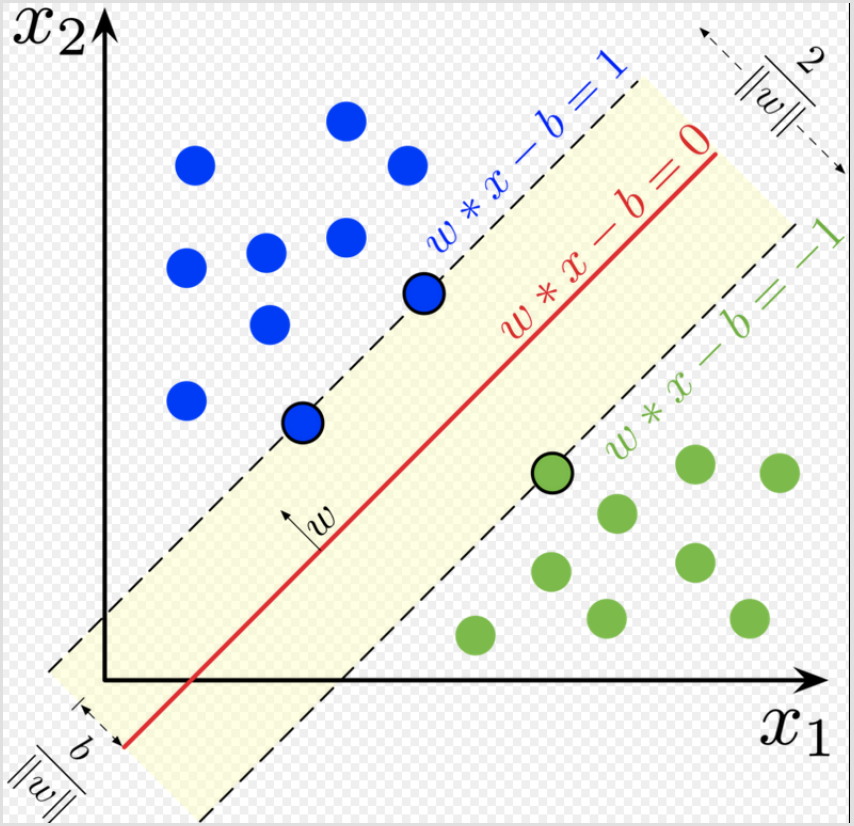

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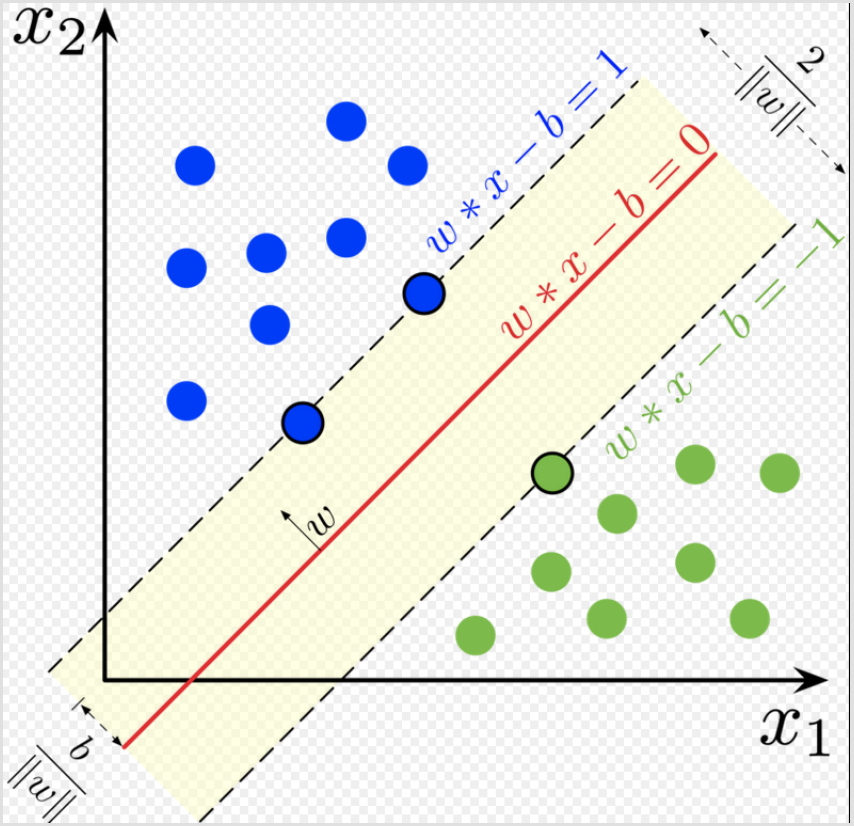

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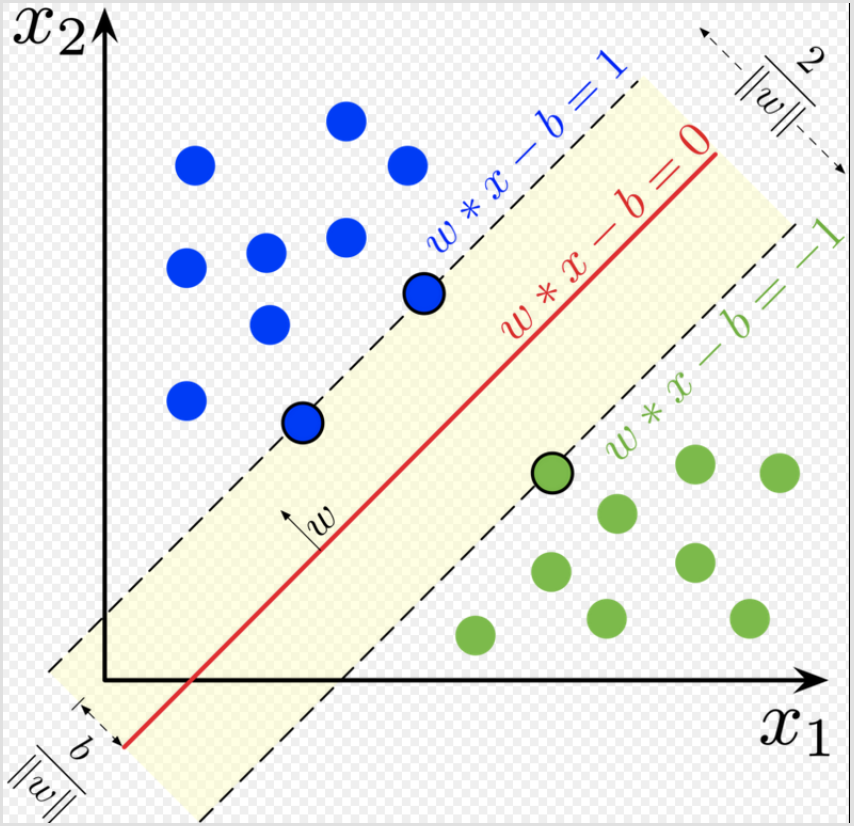

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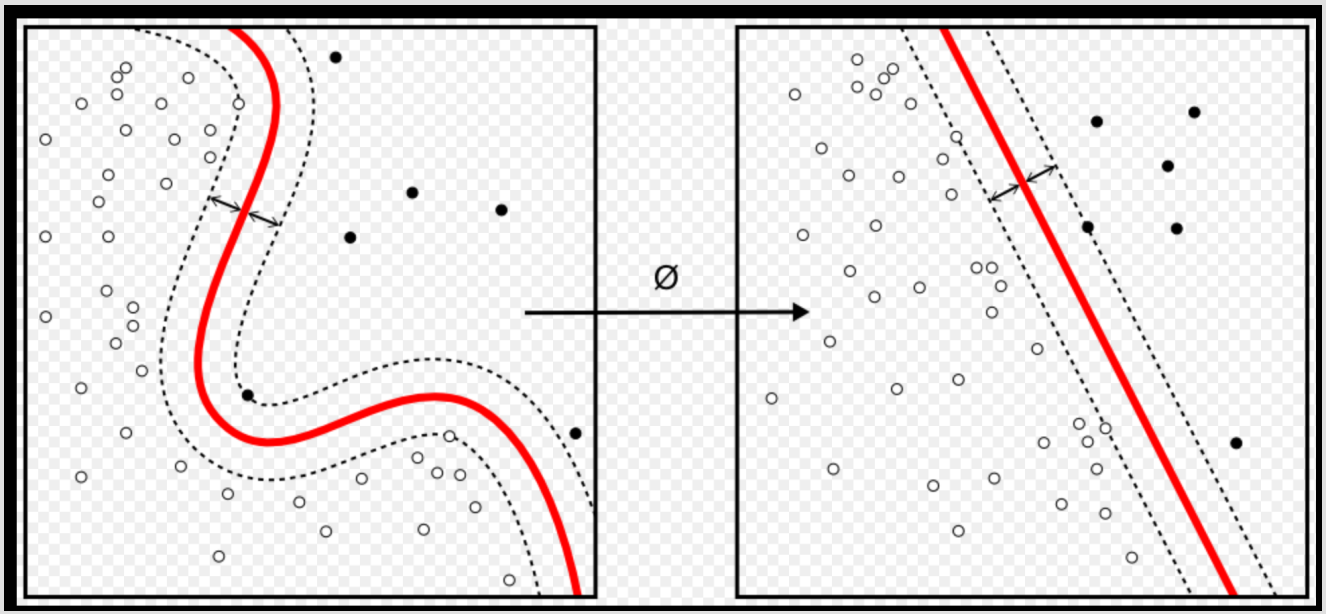

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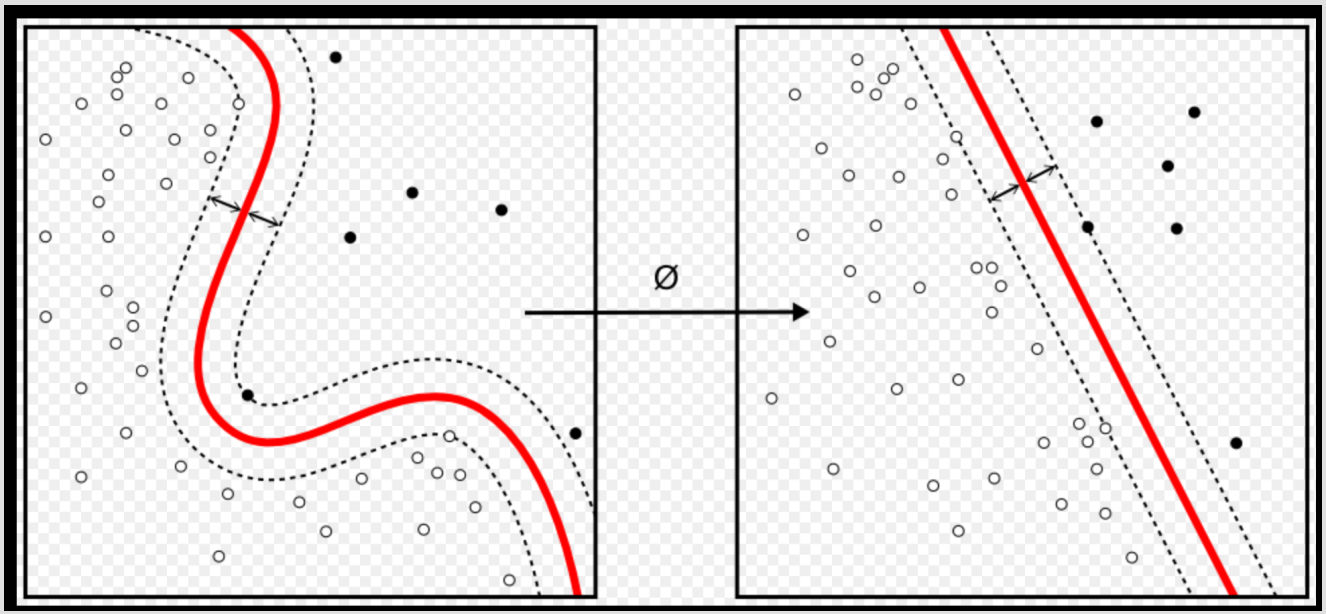

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- Linear SVM $\rightarrow$ Assume linearly separable data, no specific kernel needed

Include Linear SVM in Analysis

- Setup linear SVM in scikit

```
from sklearn.svm import LinearSVC

my_linsvm  = LinearSVC(
    max_iter = 1000, #-->Set the max. number of iterations
    C=1.0, #--> Steer performance, large / low margin
    tol=1e-6
)
```

Include Linear SVM in Analysis

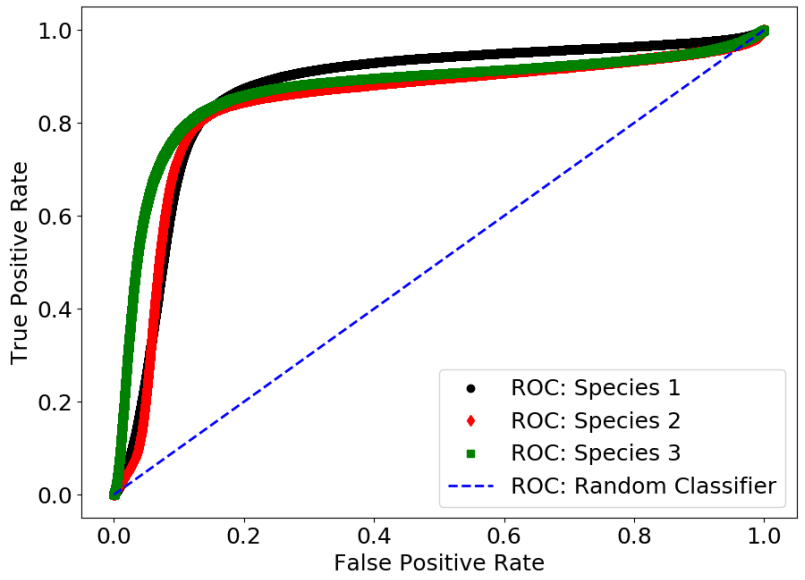
- Setup linear SVM in scikit
- Fit the data and obtain predicted labels

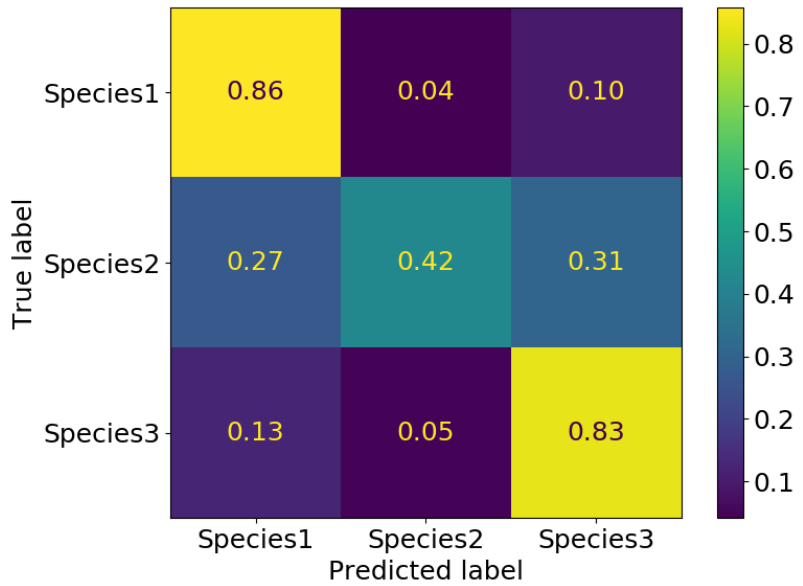
```
#Train the model:
my_linsvm.fit(x_train,y_train)

#Get the predictions:
predictions = my_linsvm.predict(X)
```

Include Linear SVM in Analysis

- Setup linear SVM in scikit
- Fit the data and obtain predicted labels
- Check performance





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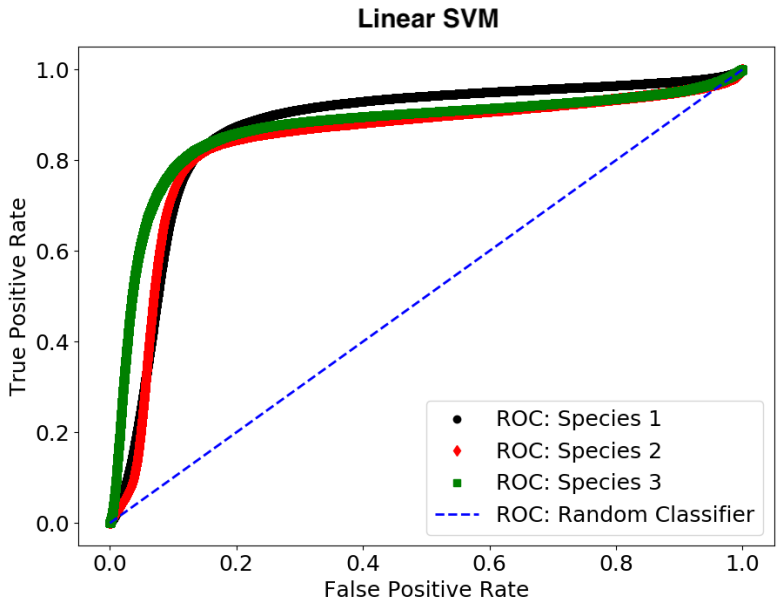

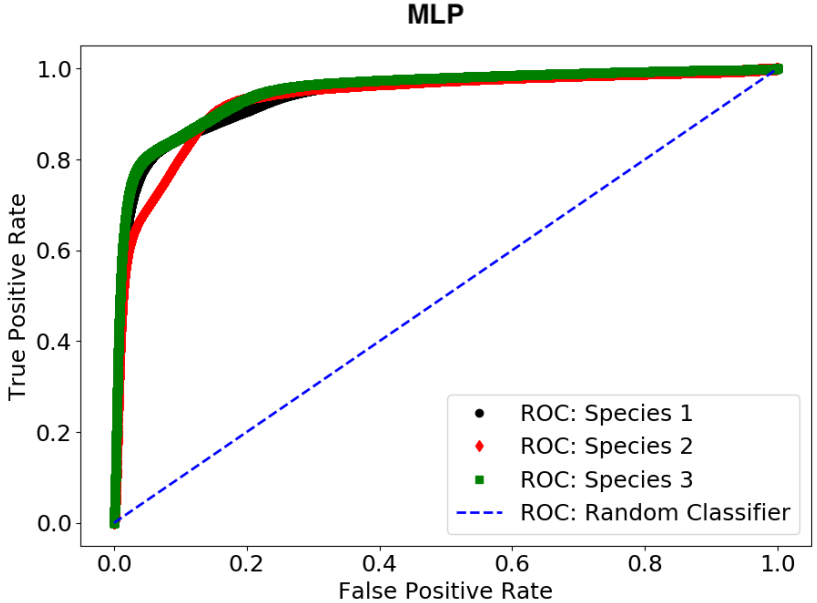

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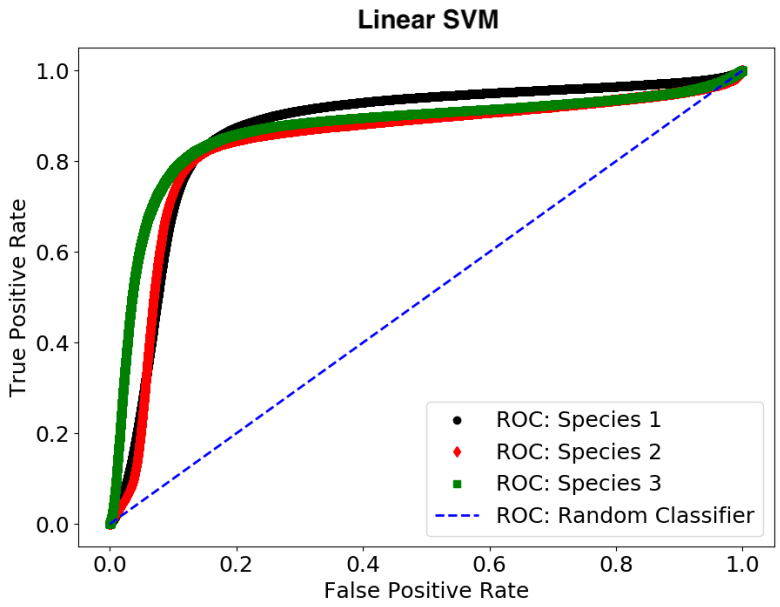

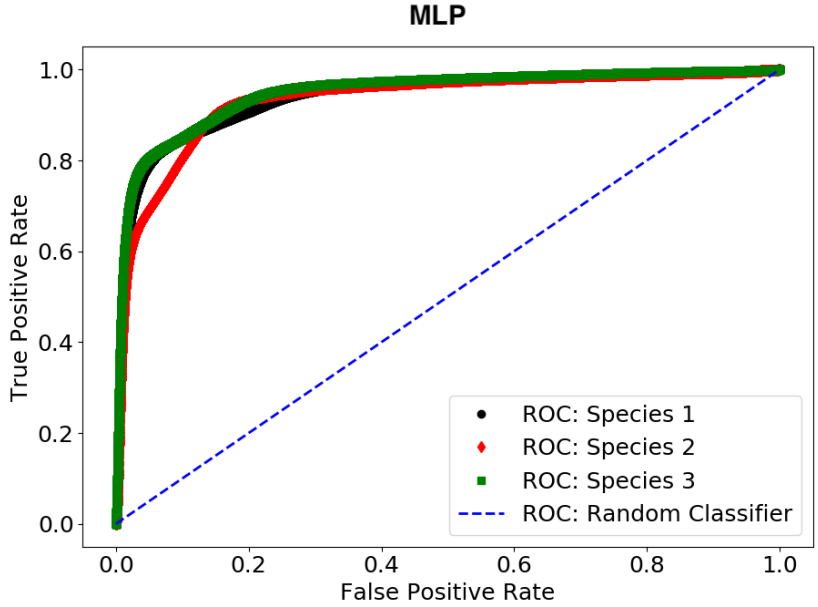

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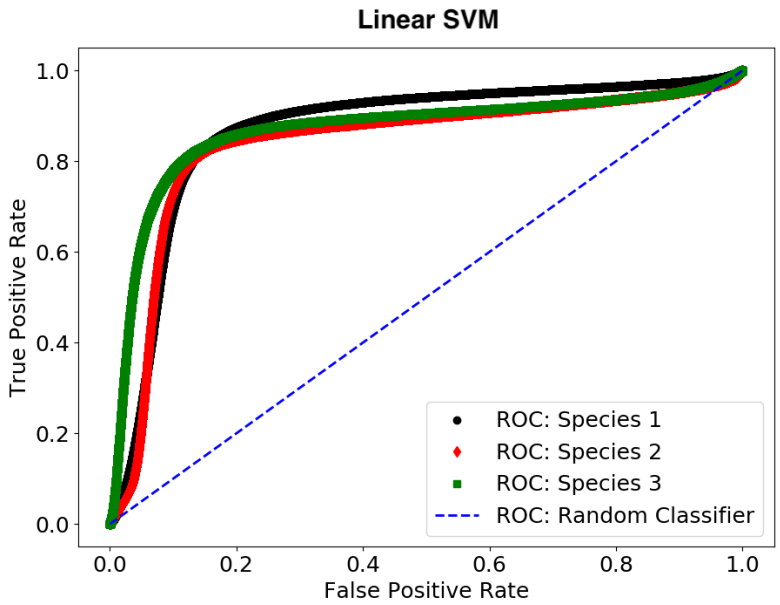

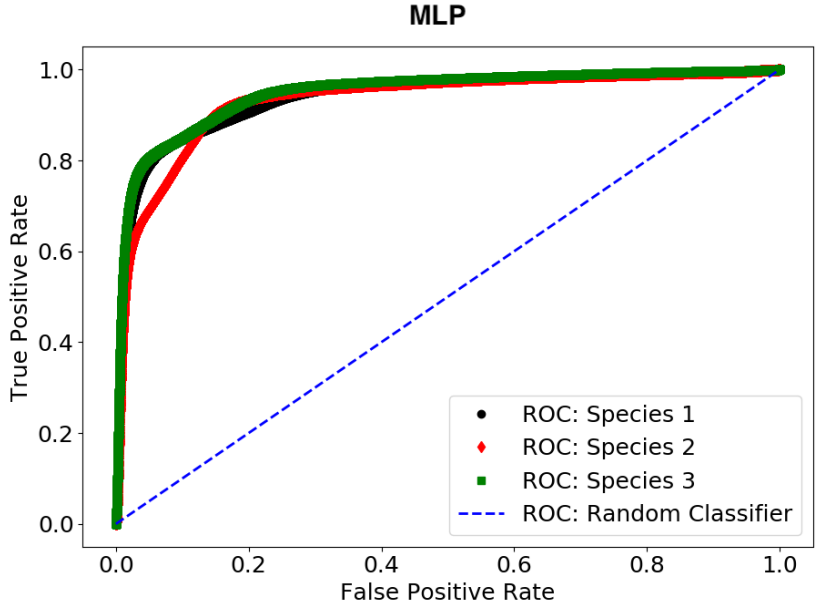

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- Is there another way to compare classifier (performances) $\rightarrow$ Evaluation metrics

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- On the following slides: introduce a few of the most common metrics

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The Purity

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- Using the basic definitions of true positive rate and false positive rate, one might rewrite the equation above to:

$$\text{Purity i} = \frac{\text{TPR(i)}}{TPR(i) + \left(\frac{1-R(i)}{R(i)}\right) \cdot FPR(i)} \tag{2}$$

with: TPR(i) / FPR(i) being the true / false positive rate for species i and: $R(i) = \sum_i \frac{\#\text{Events with species i}}{\#\text{Events}}$, the relative abundance of species i within the given data set

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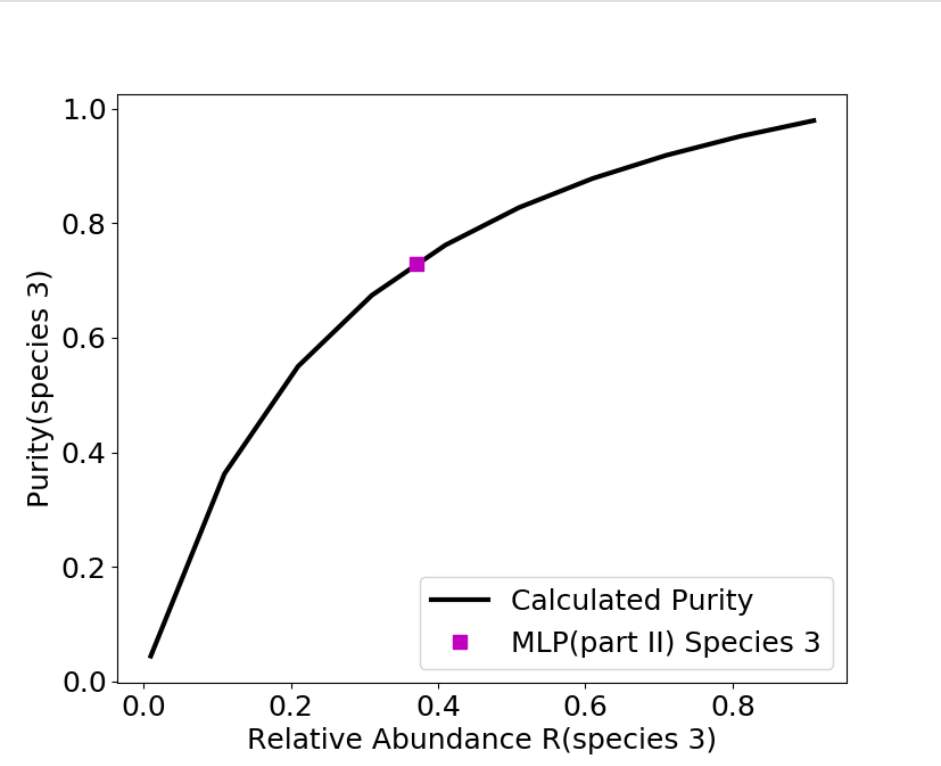

The F1-Score

- Deduced from F-measure
- The F1-Score basically folds in the true positive rate (or efficiency) and the purity

$$\text{F1-Score (species i)} = 2 \cdot \frac{\text{TPR(i)} \cdot \text{Purity(i)}}{\text{TPR(i)} + \text{Purity(i)}} \tag{3}$$

- By definition, the F1-Score also depends on the relative abundances $R(i)$

The Accuracy

- The accuracy is given by:

$$\text{Accuracy} = \frac{1}{\#\text{Events}} \sum_{i}^{\#\text{Species}} \#\text{Events with species i \& identified as i} \quad (4)$$

$$= \frac{1}{\#\text{Events}} \sum_{i}^{\#\text{Species}} \text{TPR(i)} \cdot N(i) \quad (5)$$

$$= \sum_{i}^{\#\text{Species}} \text{TPR(i)} \cdot R(i) \quad (6)$$

- Or: Accuracy $\propto$ Tr(confusion matrix)
- Again, the relative abundance is folded in
- The accuracy is less reliable on highly imbalanced data, i.e. R(j) >> R(i)

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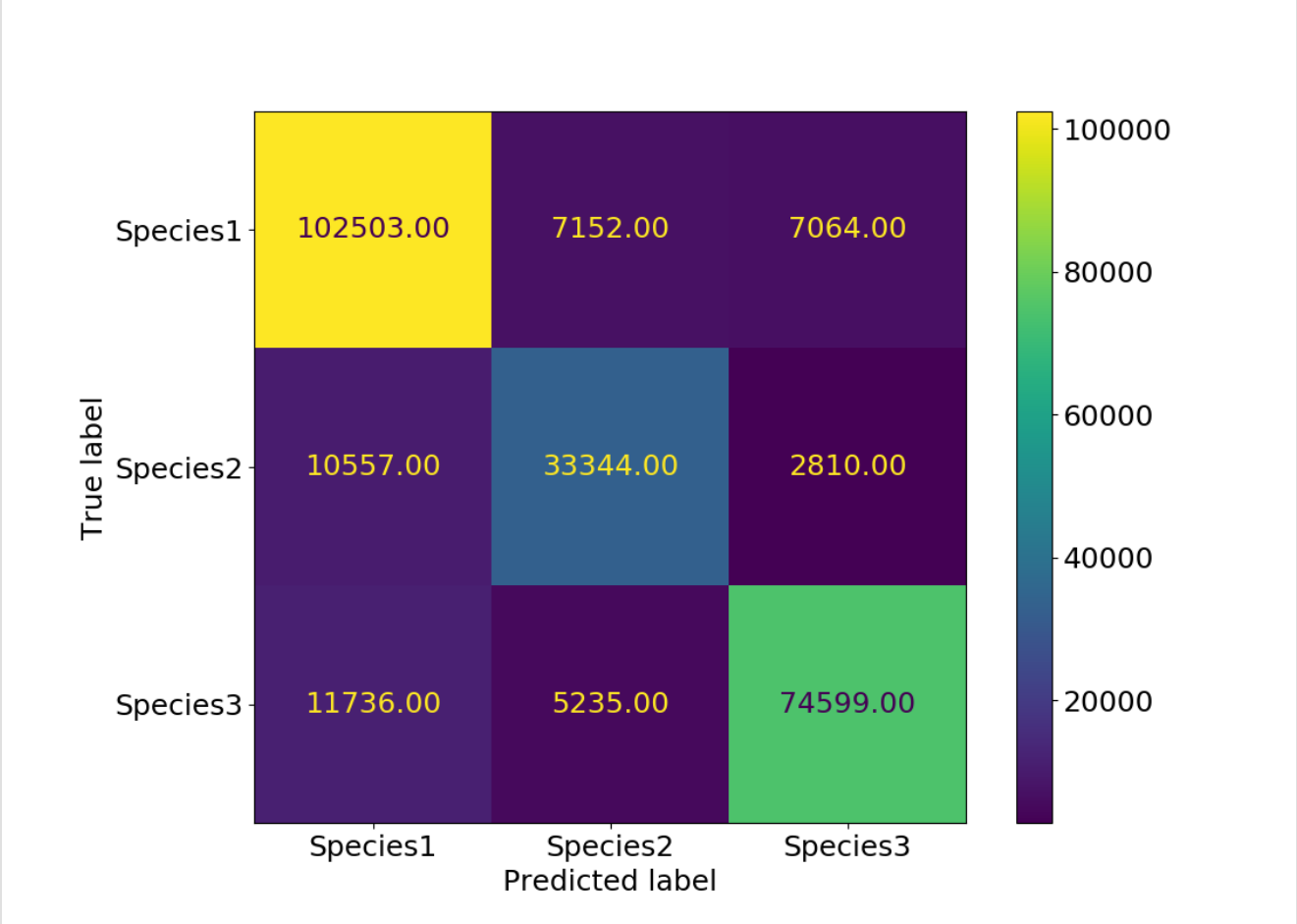

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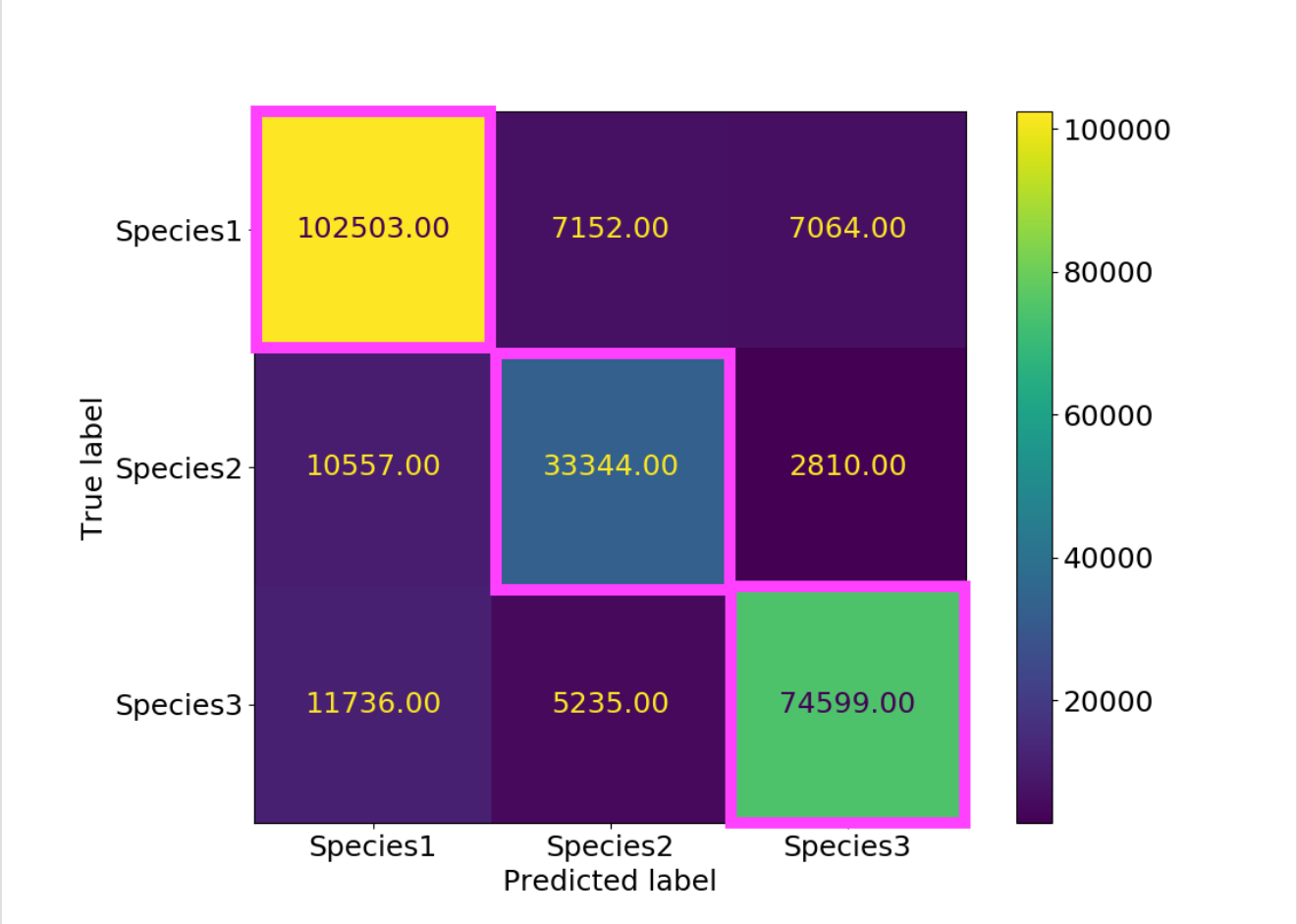

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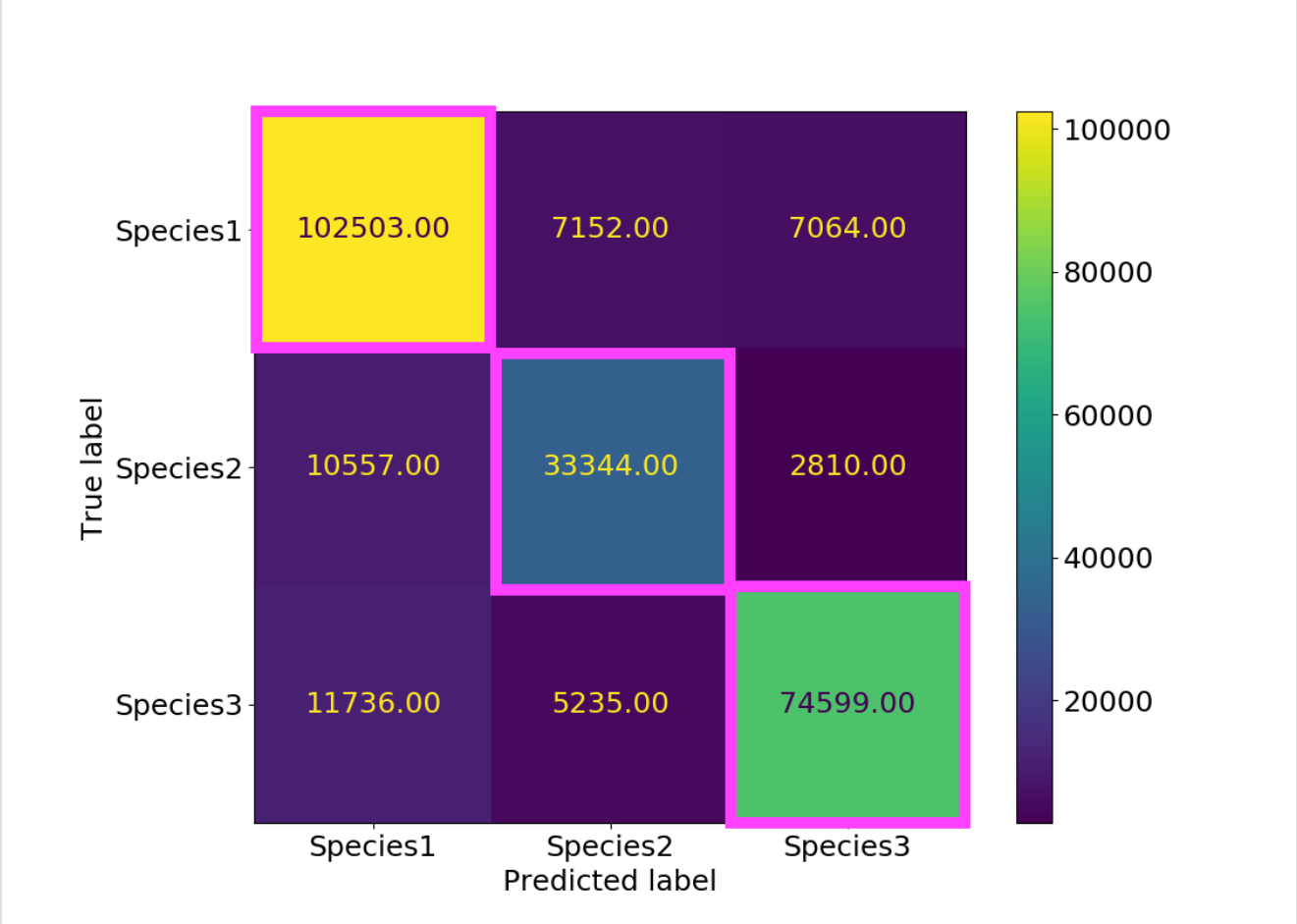

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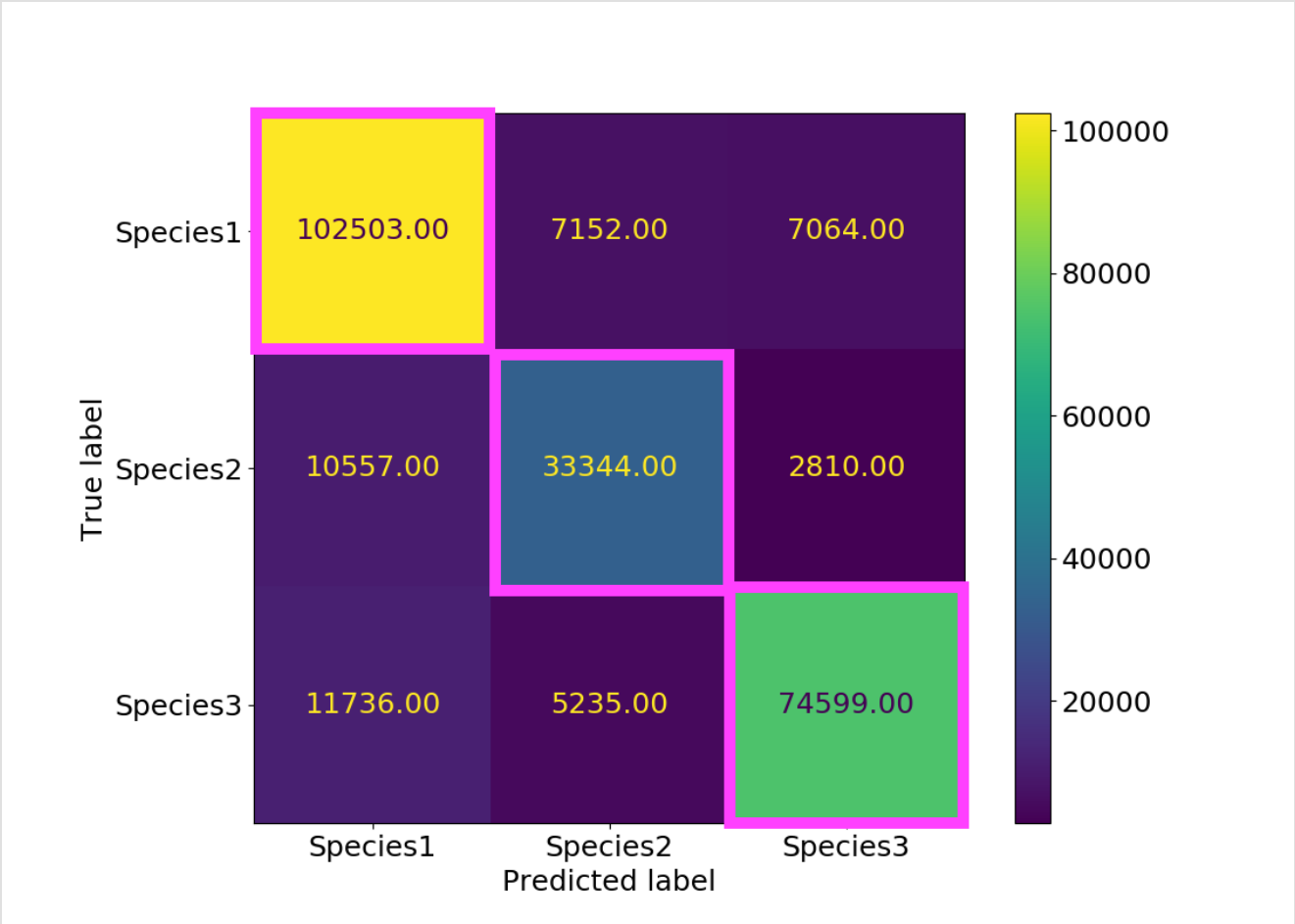

- The trace of this matrix is: TR = 102,503 + 33,344 + 74,599 = 210,446
- The total number of events in the given data set is: #Events = 255,000
- Using Eq. 4 from slide 14 yields: Accuracy = TR / #Events ≈ 82%
  → consistent with the value reported by scikit

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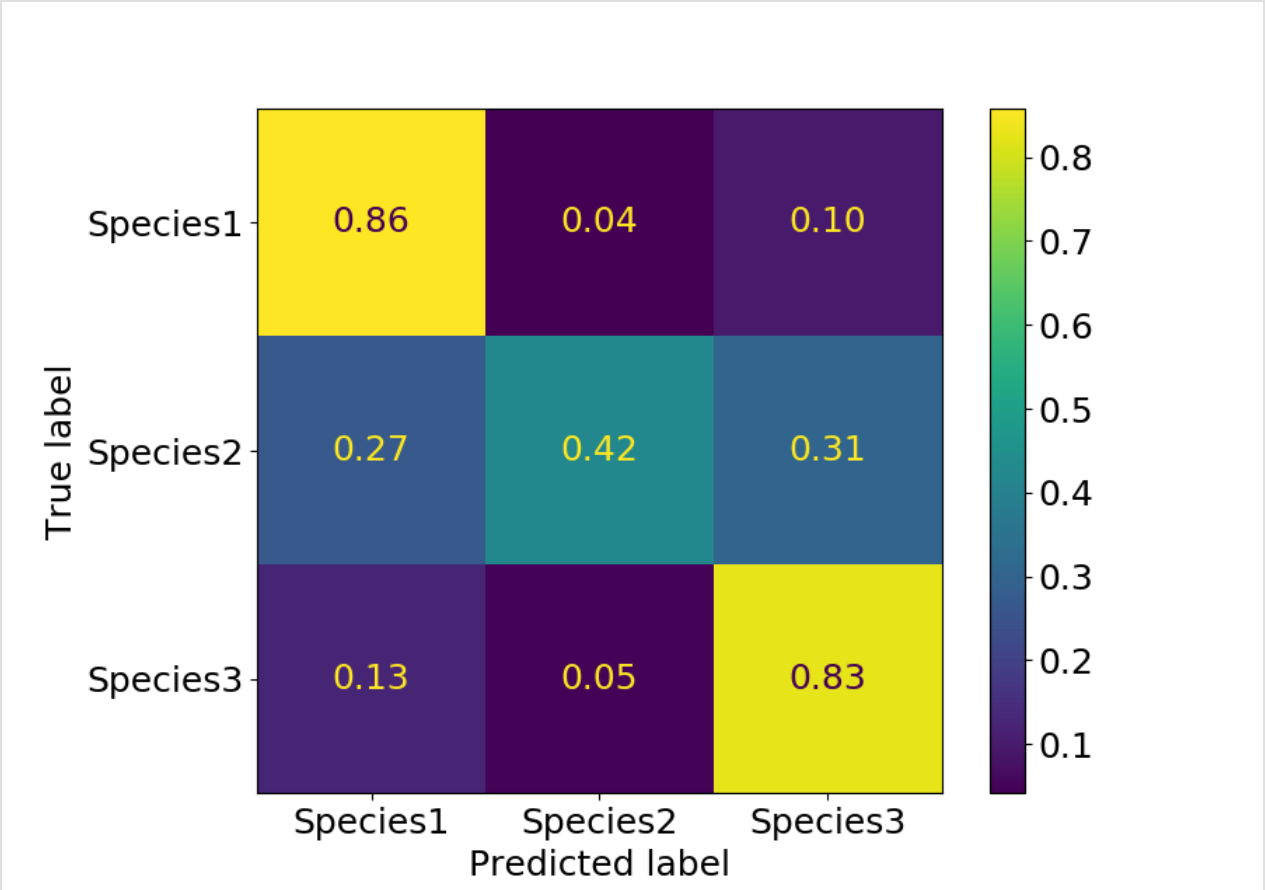

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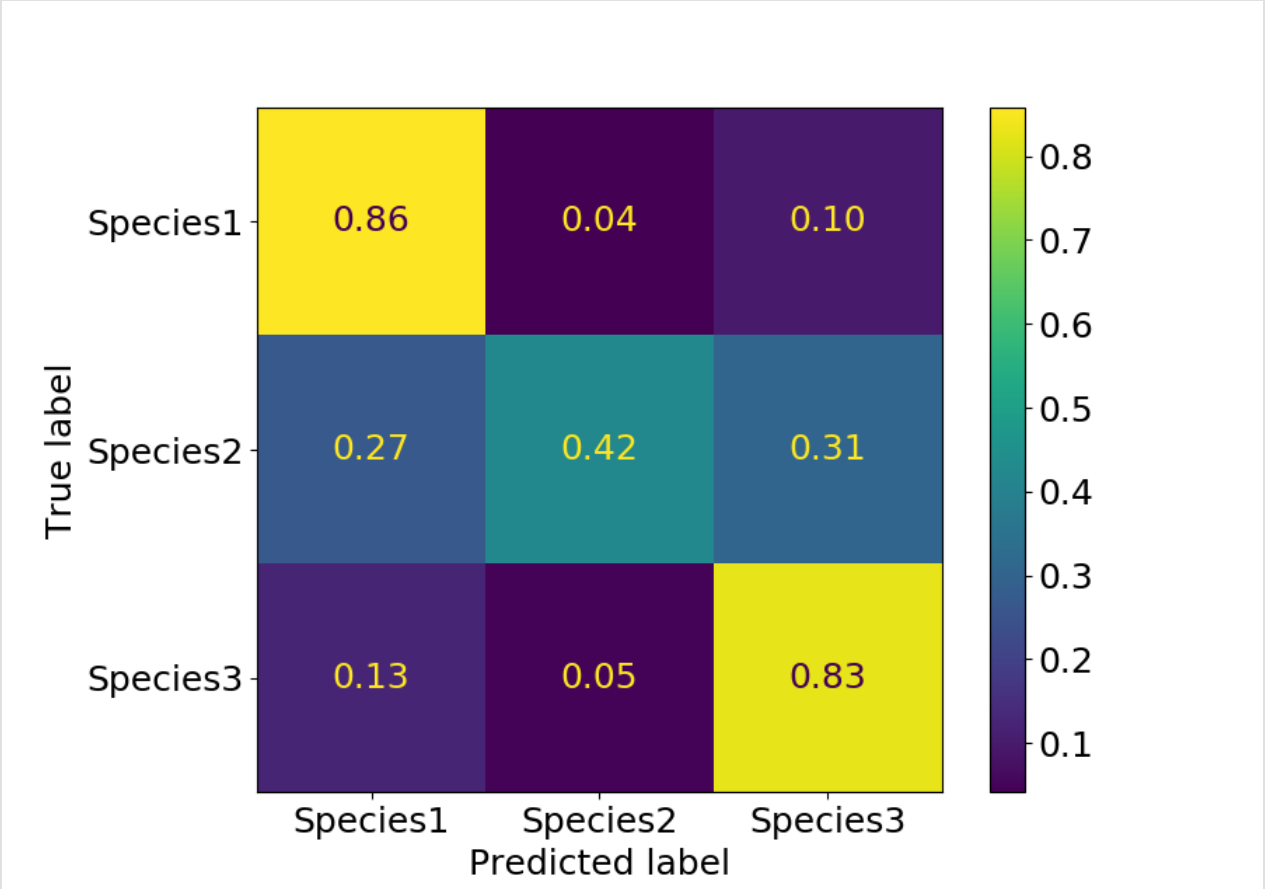

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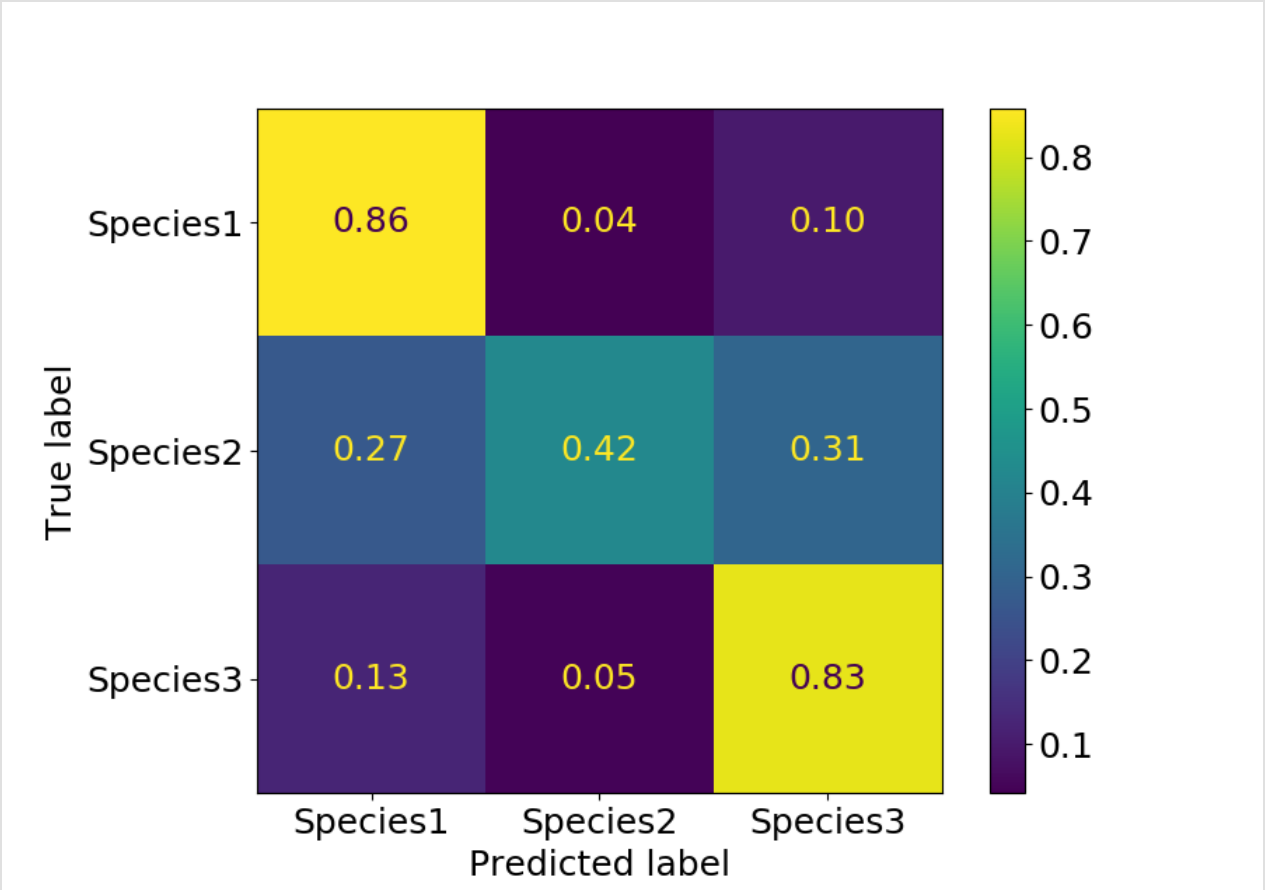

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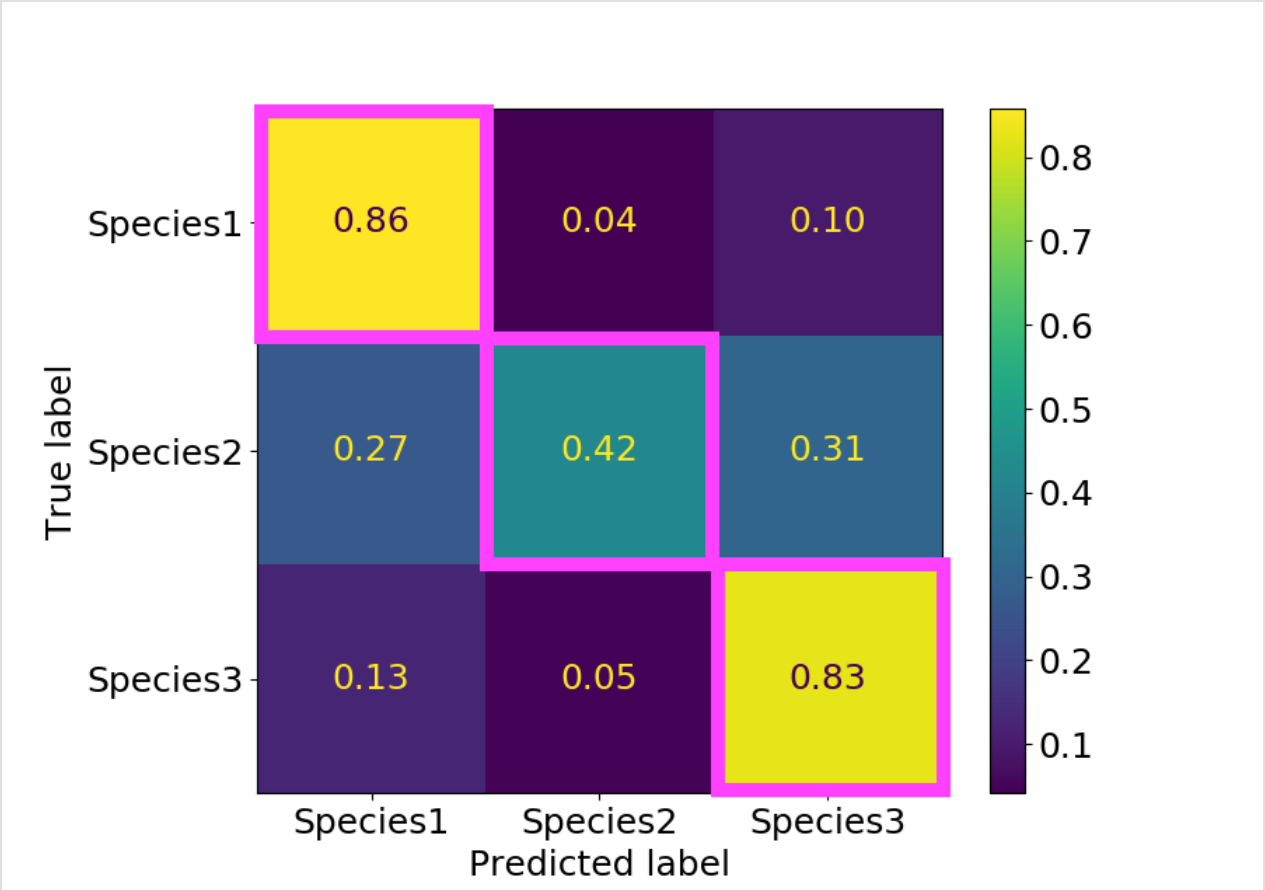

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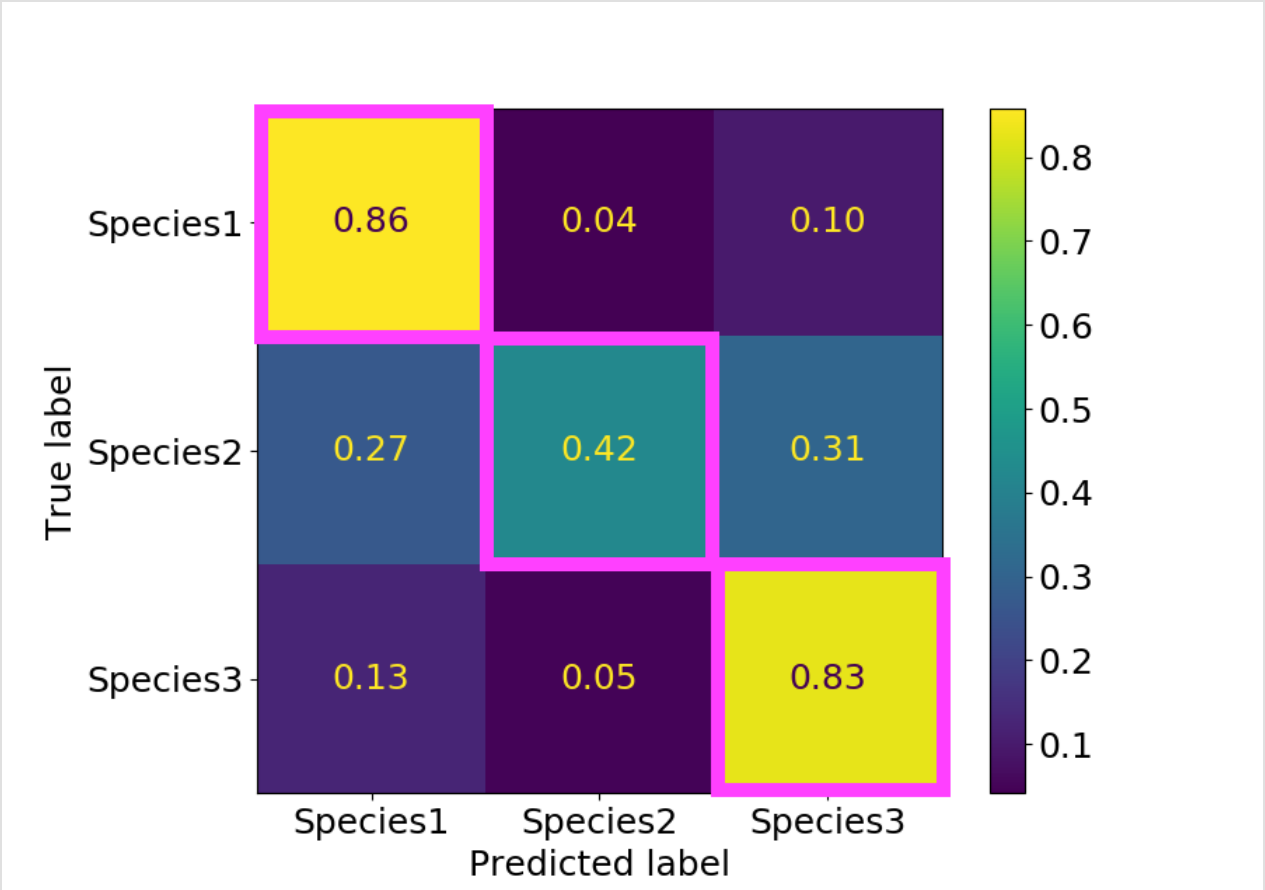

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- Note that contribution for species 2 is suppressed due to R(2)

The Matthews Correlation Coefficient (MCC)

- Like the accuracy, the MCC can be computed from entries within the (unnormalized) confusion matrix:[8]

$$\mathrm{MCC} = \frac{\sum_k \sum_l \sum_m (C_{kk} C_{lm} - C_{kl} C_{mk})}{\sqrt{\sum_k (\sum_l C_{kl})(\sum_{k' \neq k} \sum_{l'} C_{k'l'})} \cdot \sqrt{\sum_k (\sum_l C_{lk})(\sum_{k' \neq k} \sum_{l'} C_{k'l'})}} \tag{7}$$

- In a very simplified picture, the MCC combines the true positive rate, false positive rate and purity[9]
- The MCC is a common / preferable choice for imbalanced data

[8] Formula taken from **wikipedia**

[9] This is exact true for binary classification

Example

- Compare performance metrics of mlp and linear svm on the given data set

Model	F1-Score	Accuracy	MCC
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  - ... on which information you would like to retrieve (e.g. care more about purity, or efficiency, or overall classification performance?)

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Random Forest	Thresholds in trees	#Trees, depth of each tree,...

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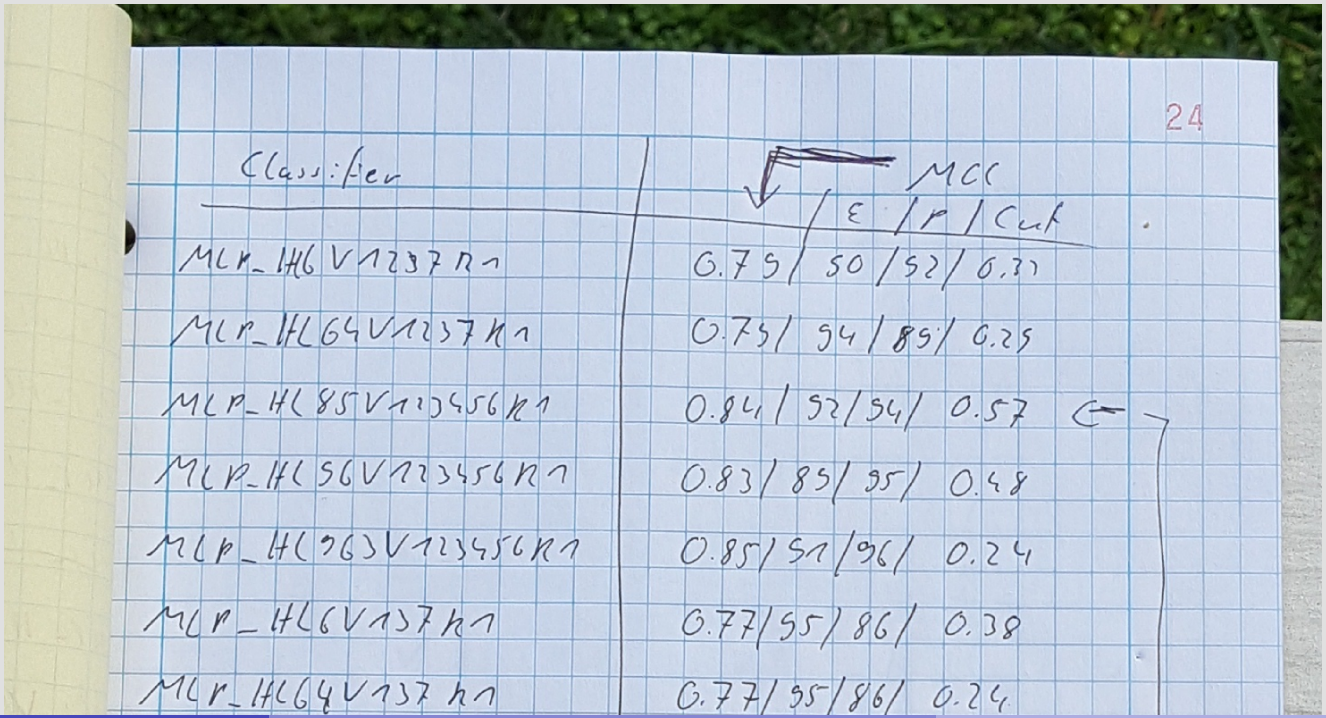

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  - ...
- No matter which method you decide to use $\rightarrow$ Always include a validation data set

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- Look again at the classification data (three species, defined by three features each)

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Epochs	100, 200, 700
Learning Rate	0.005, 0.01, 0.02
Architecture	(5), (10), (5,3)

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$\Rightarrow$ 4 hyper parameters with 3 settings each $\rightarrow 3^4 = 81$ settings to test
$\rightarrow$ This might take a while...

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Setting up and performing the Grid Search

- Split data into training and validation sets

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```
from sklearn.model_selection import train_test_split

#Load the DataFrame:
data = '/Volumes/BunchOfStuff/classifier_testData/fsu_ml_data3.csv'
data_df = pd.read_csv(data)

#Get features and labels:
X = data_df[['var1','var2','var3']].values
Y = data_df['label'].values

#Divide data into training and validation sets
x_train, x_val, y_train, y_val = train_test_split(
        X, #--> features
        Y, #--> targets
        test_size=0.25, #--> Percentage of data that is used for validation
        random_state=0)
```

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```
def setup_mlp(architecture,n_epochs,act_func,l_rate):
        my_mlp = MLPClassifier(
        hidden_layer_sizes=architecture, #--> Updated for each param. setting
        activation=act_func, #--> Updated for each param. setting
        solver='sgd',
        shuffle=True,
        validation_fraction=0.1, #--> part of the training data
        #is used for early stopping
        early_stopping=True,
        max_iter = n_epochs, #--> Updated for each param. setting
        learning_rate_init=l_rate, #--> Updated for each param. setting
        learning_rate='invscaling', #--> Decreasing learning rate
        #will be discussed later
        warm_start=True,
        tol=1e-6
    )

    return my_mlp
    #--> In our example, this function will be called 81 times...
```

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  $\Rightarrow$ Accuracy, Purity, log-loss, Matthews Correlation Coefficient,...
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a) Train the mlp on the training data

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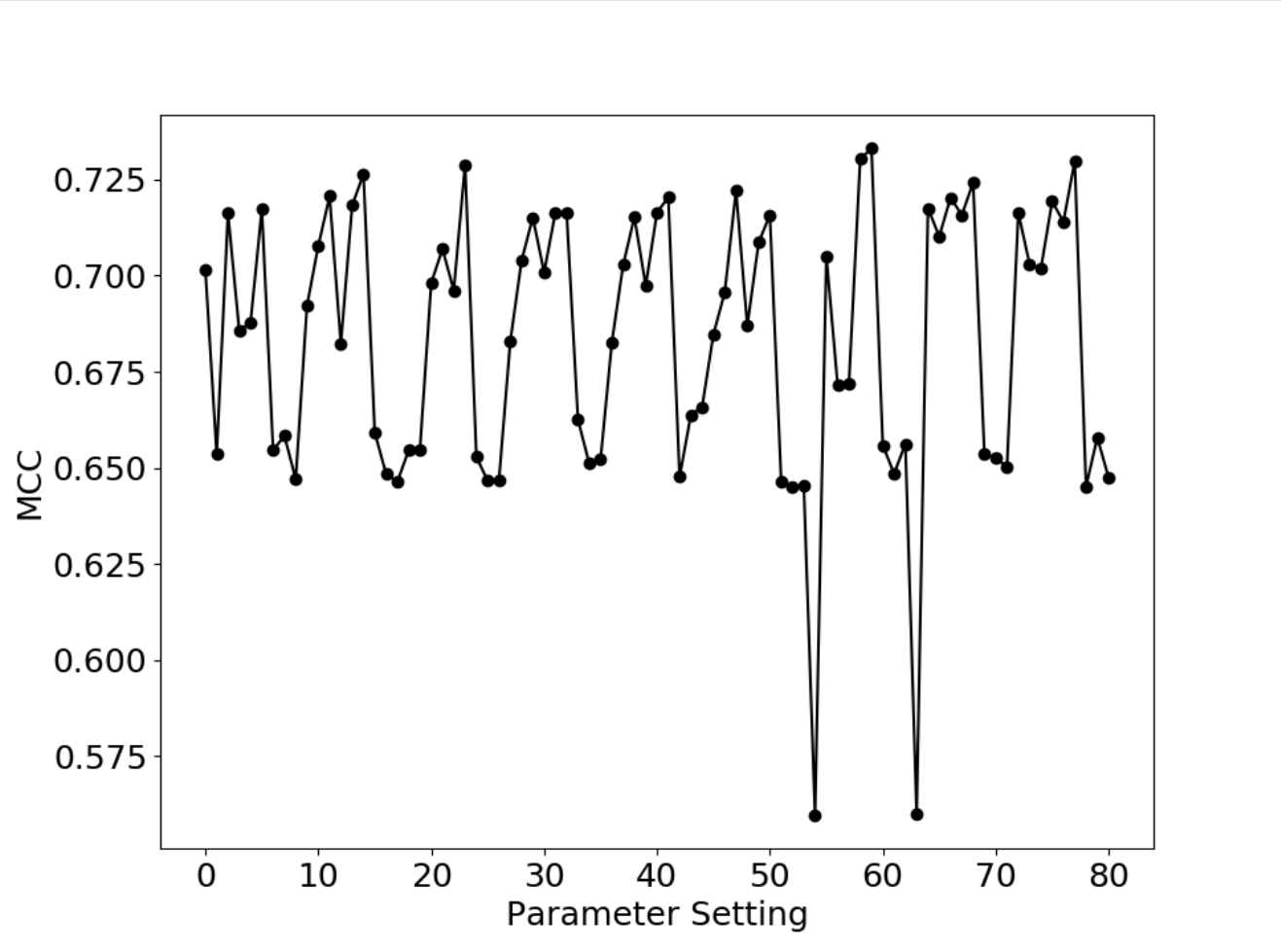
- Finally, pick algorithm that shows highest[11] performance

[11] In some cases not the best choice

Results of MLP Parameter Grid Search

- Check performance[12] vs. parameter setting

  $\leftrightarrow$ Understand model behavior with respect to parameter settings / ranges



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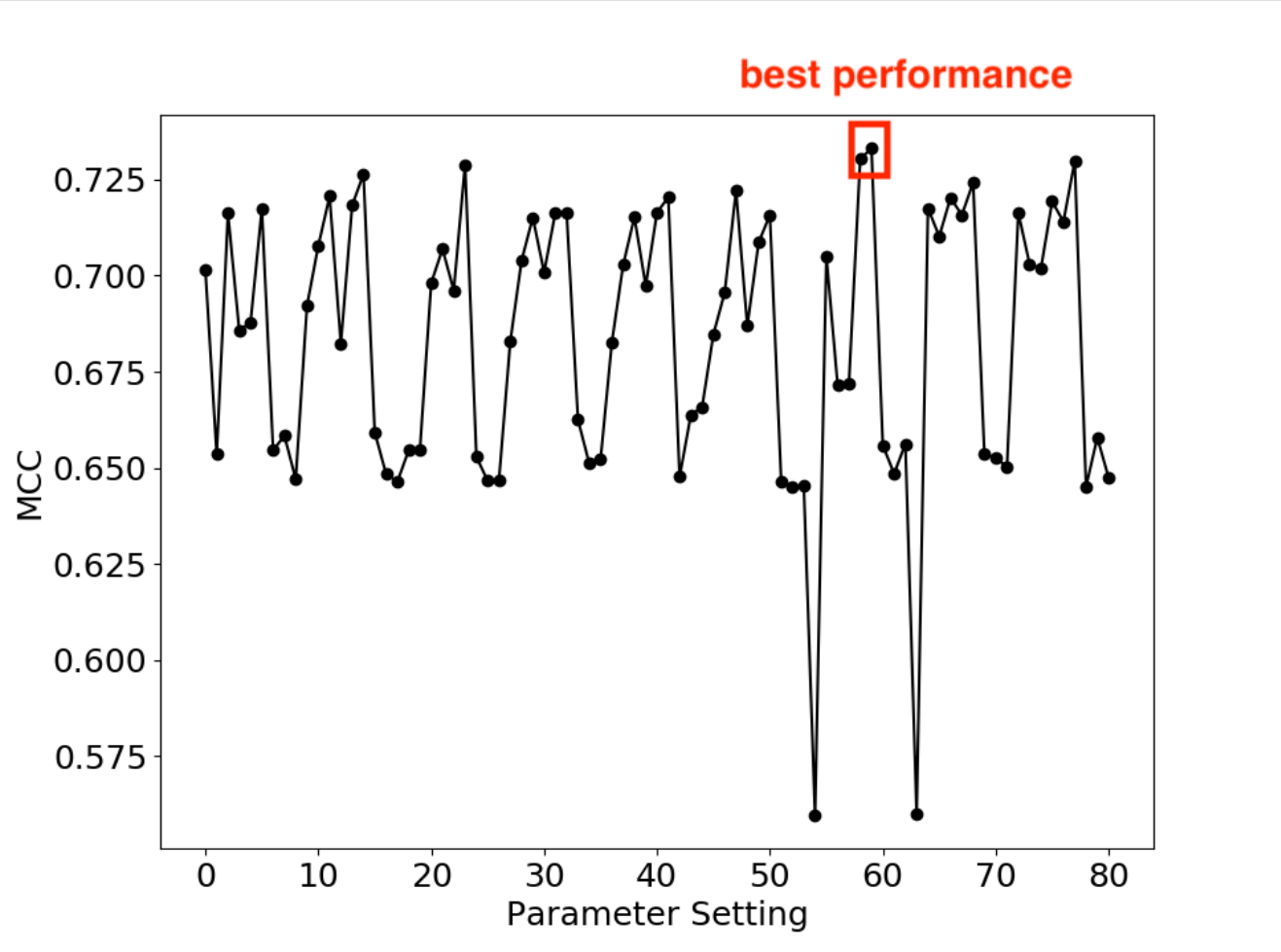

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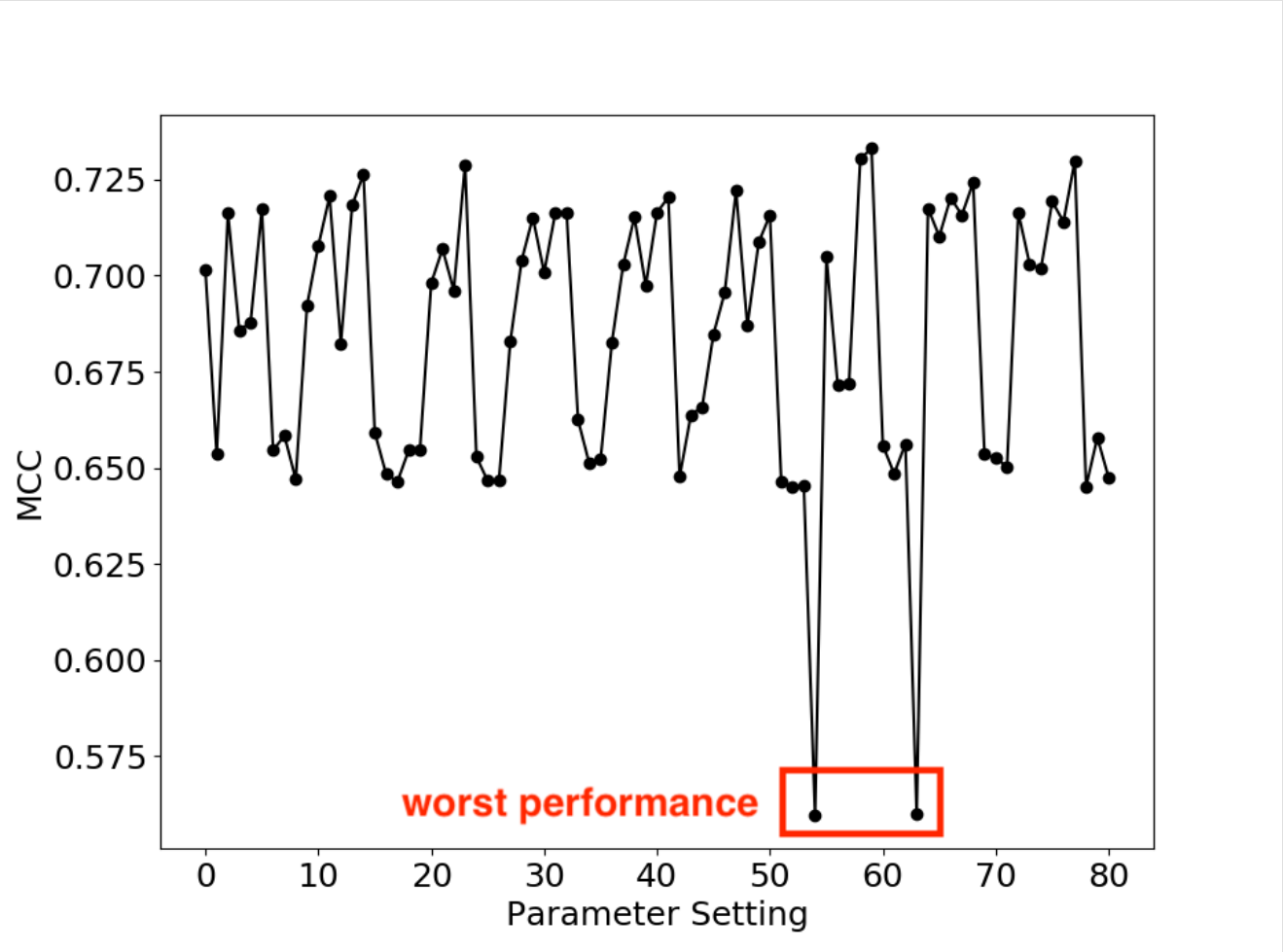

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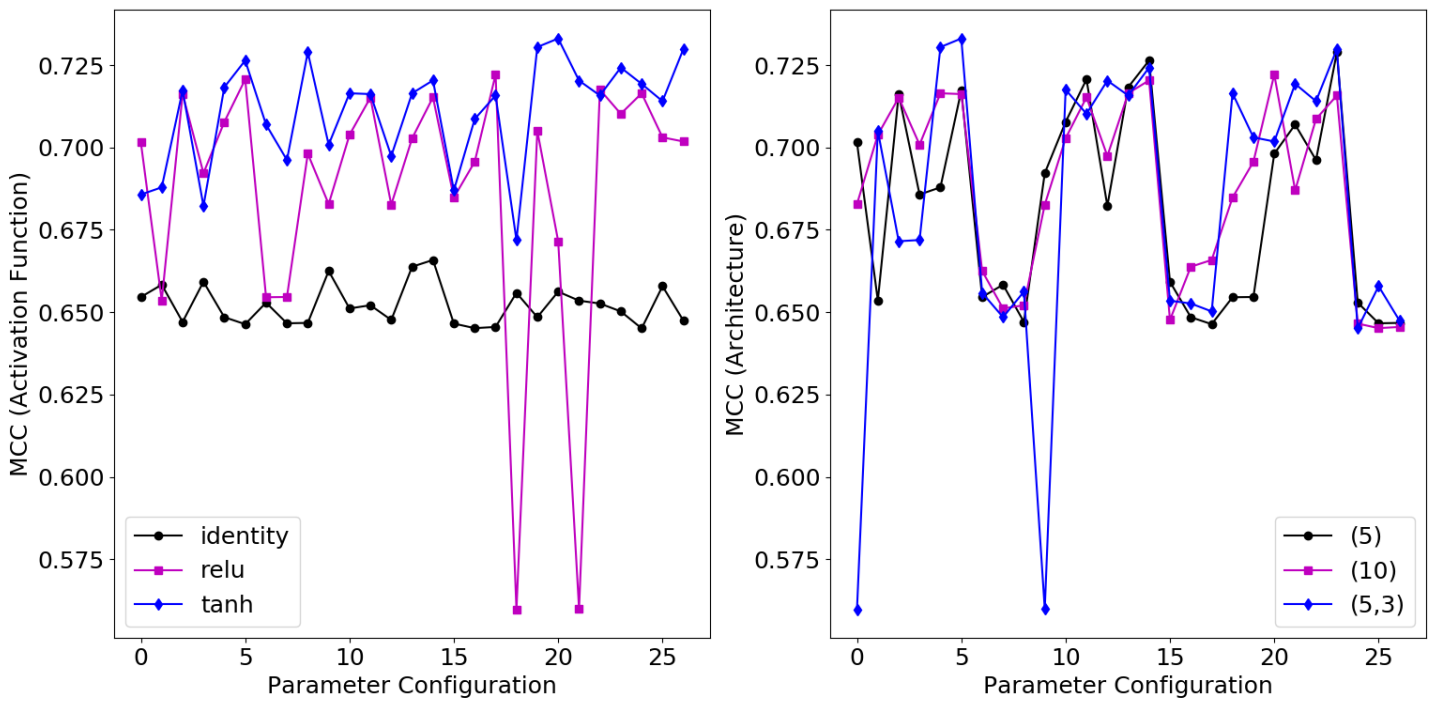
- Look at performance for specific hyper parameter settings

  $\leftrightarrow$ Study significance of parameter with respect to performance



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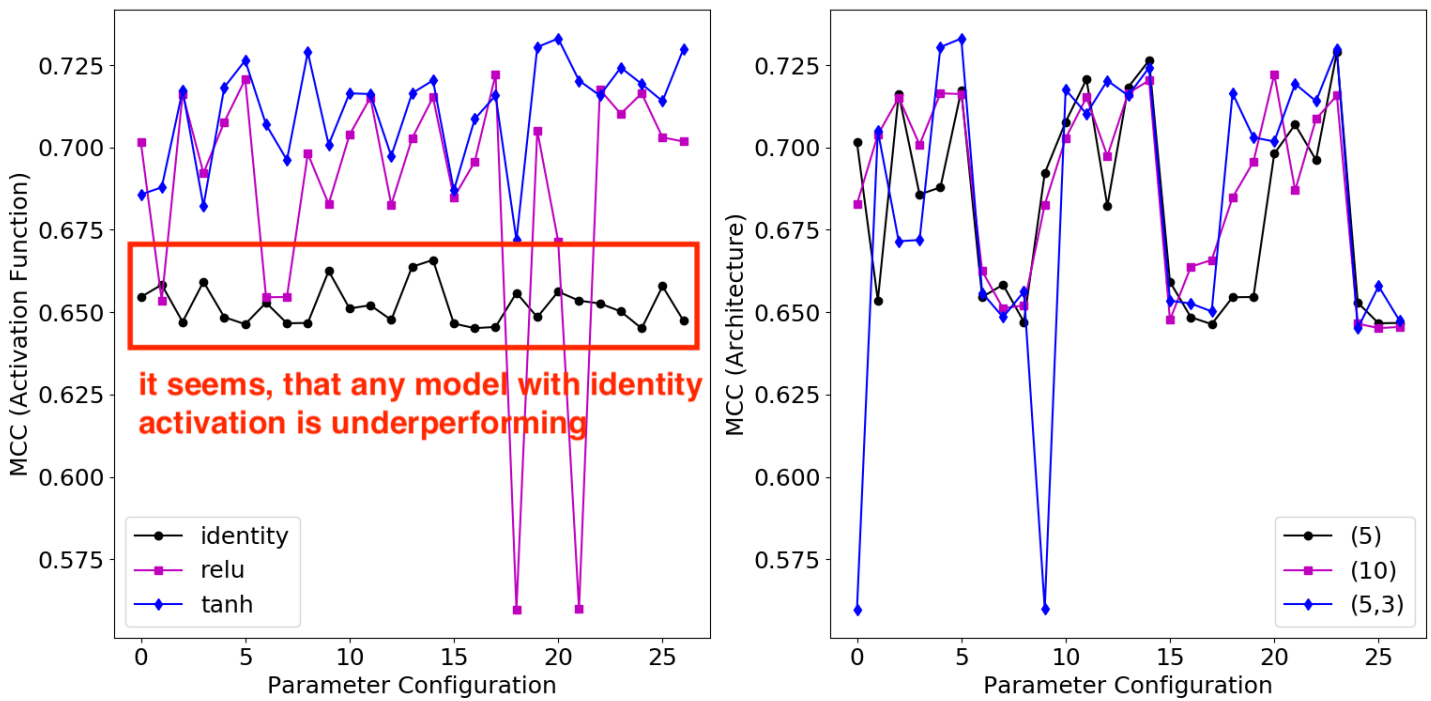

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- Check performance[12] vs. parameter setting
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- Compare individual models

  $\leftrightarrow$ Look for striking differences

Architecture	Max. # Epochs	Learning rate	Act. Func.	MCC
(5,3)	100	0.005	relu	0.56
(5,3)	100	0.05	tanh	0.73

[12] Use the Matthews Correlation Coefficient (MCC) here

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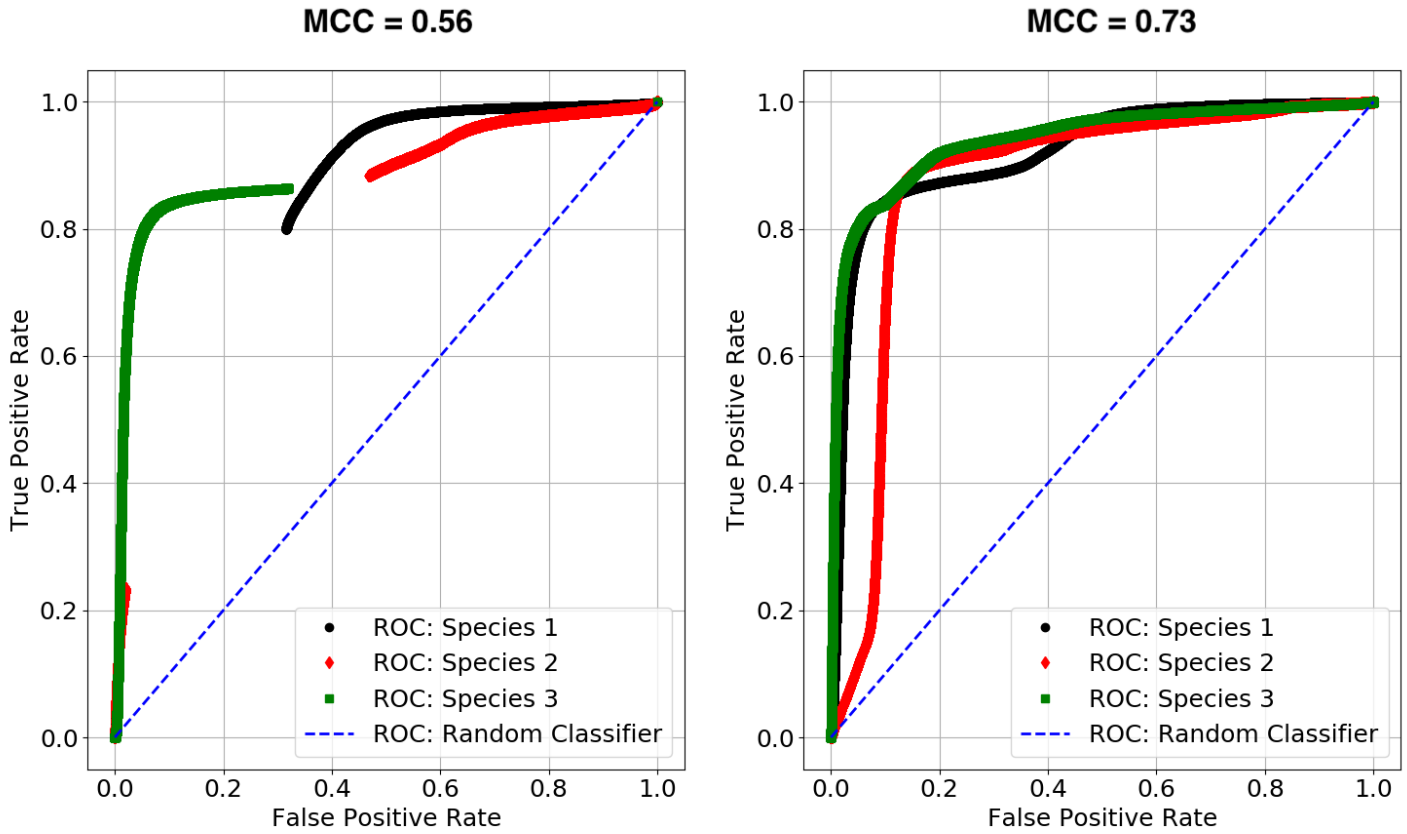

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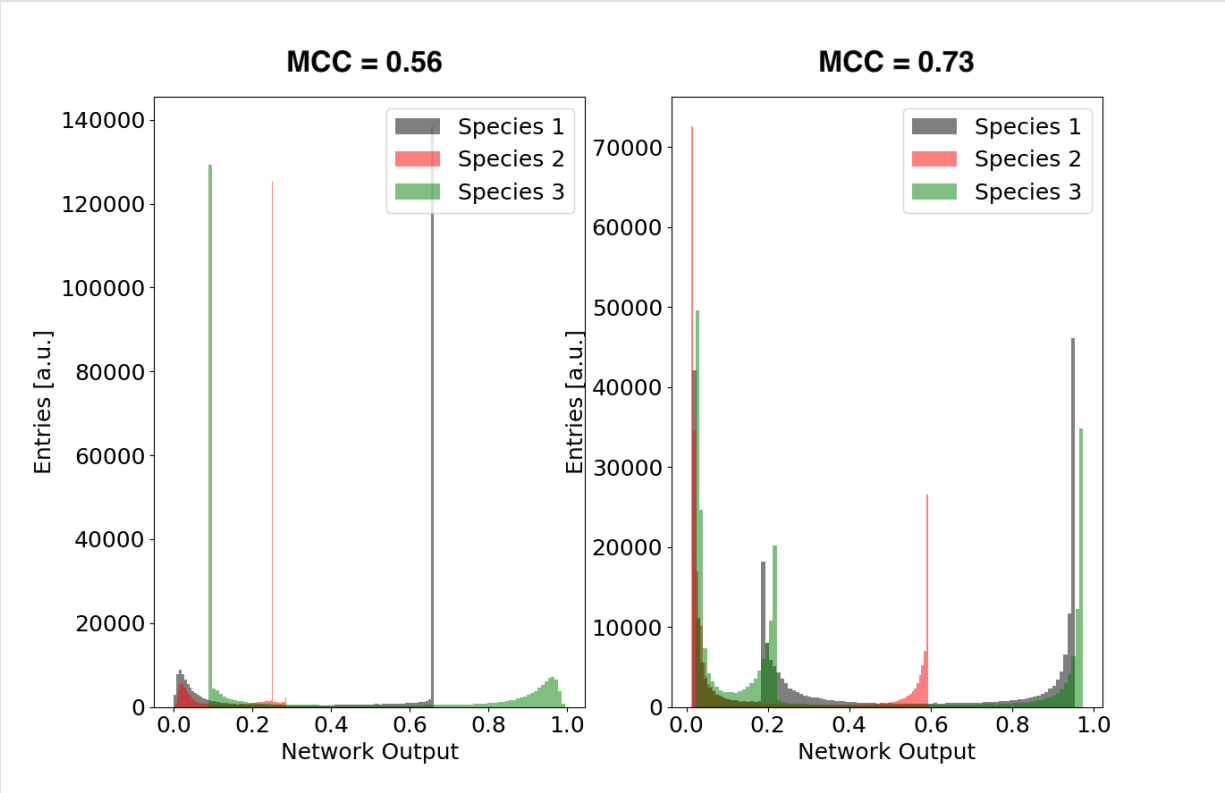

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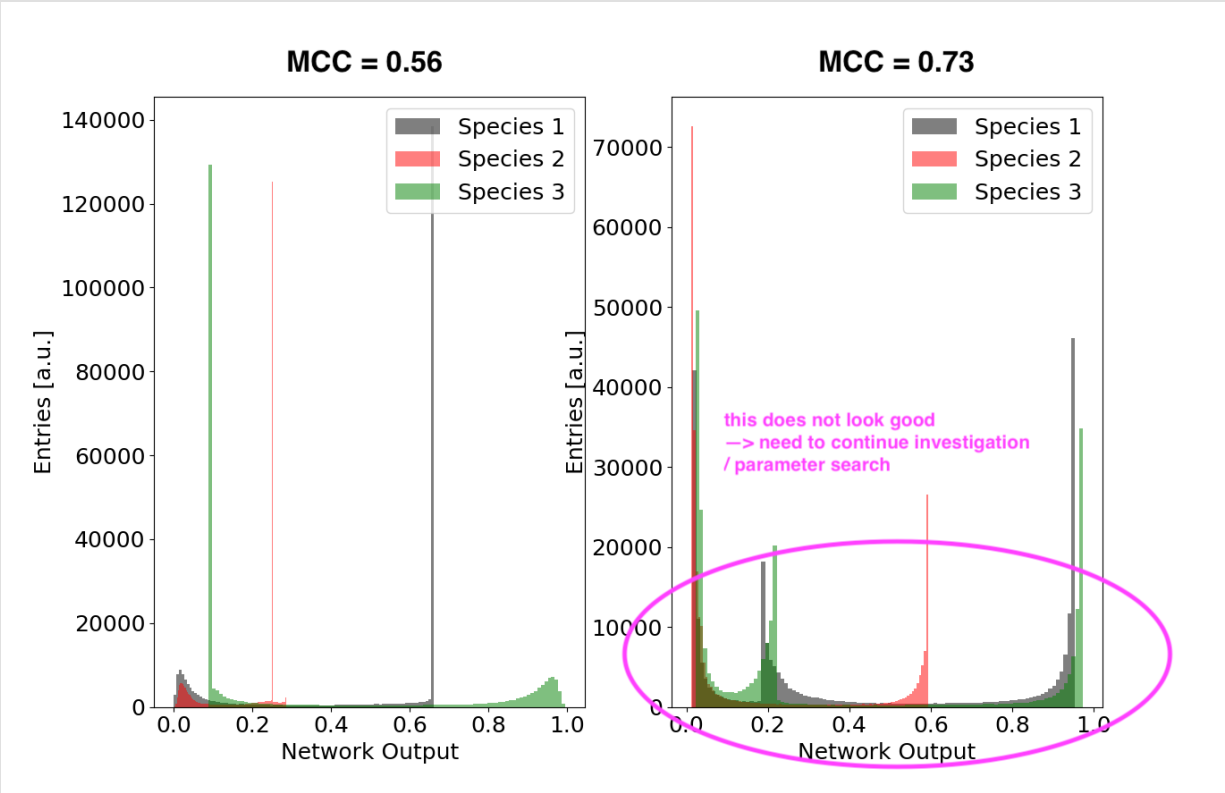

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  - No guarantee that optimal model is found within the specified limits

$\Rightarrow$ It might happen that you search for a long time, without finding the proper settings

- Grid search is helpful, if you now your model pretty well and / or have somewhat narrowed down the individual parameter limits $\Rightarrow$ Fine tuning

Summary Part III

- Briefly discussed two more classification algorithms
  - Random Forest classifier
  - Linear support vector machine
- Discussed performance evaluation metrics
  - Purity, F1-Score, accuracy and MCC
  - These are NOT all available metrics $\rightarrow$ There are many more which are frequently used (i.e. AUC)
- Hyper Parameter Optimization (HPO)
  - Tune model on given data set
  - Different approaches available
  - Discussed simple grid search
- Next part:
  - A few more words on HPO
  - Transition to deep learning