



# Deep Layers

WORKSHOP / ARTIFICIAL INTELLIGENCE

20. - 21. 9. 2022

Institute of Scientific Instruments of the Czech Academy of Sciences  
Kralovopolska 147, Brno, Czech Republic

Registration (free, but mandatory) | [www.isibrno.cz/deep](http://www.isibrno.cz/deep)



# Machine Learning Elements II – Model training

How to devide, preprocess data and build basic ML models

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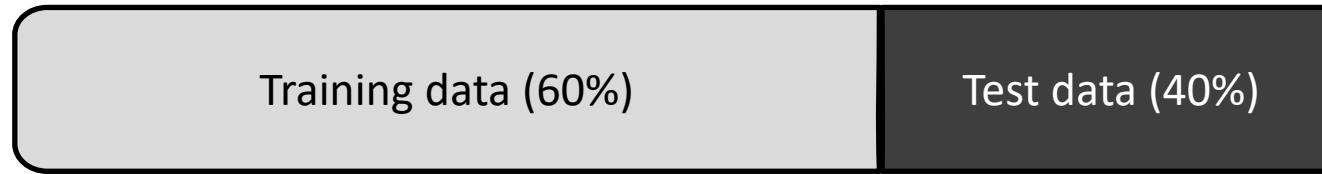
You are welcome to experiment with dataset during the lesson.

QR code link to COLAB NOTEBOOK :  
(Or through <https://www.isibrno.cz/deep/>)



# 1. Splitting data

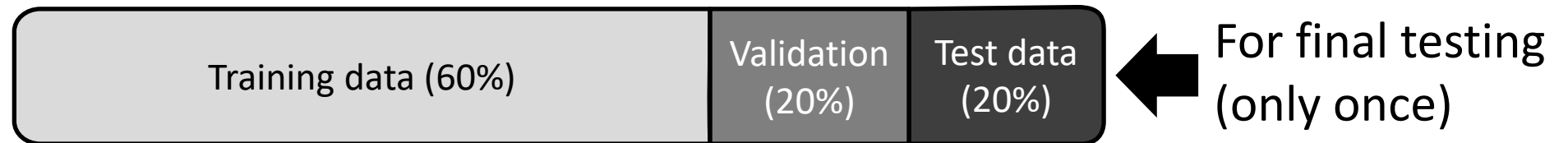
Split to training & testing data:



Link to COLAB NOTEBOOK:



More correctly (and definitely, for DL) it should be:

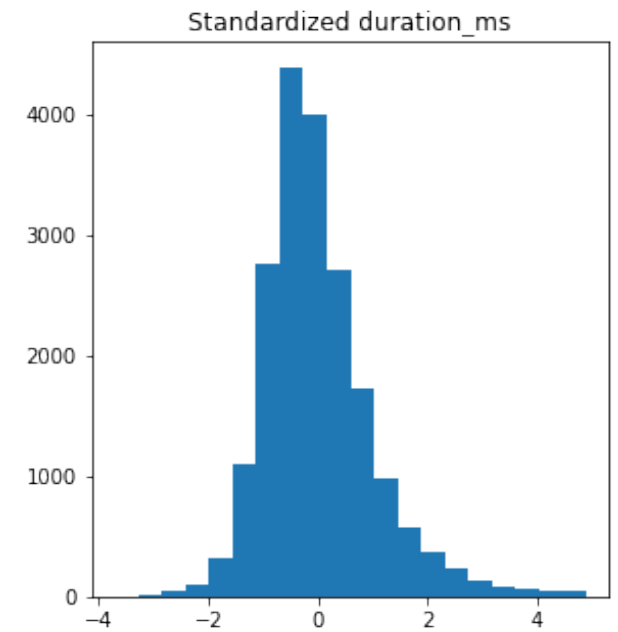
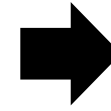
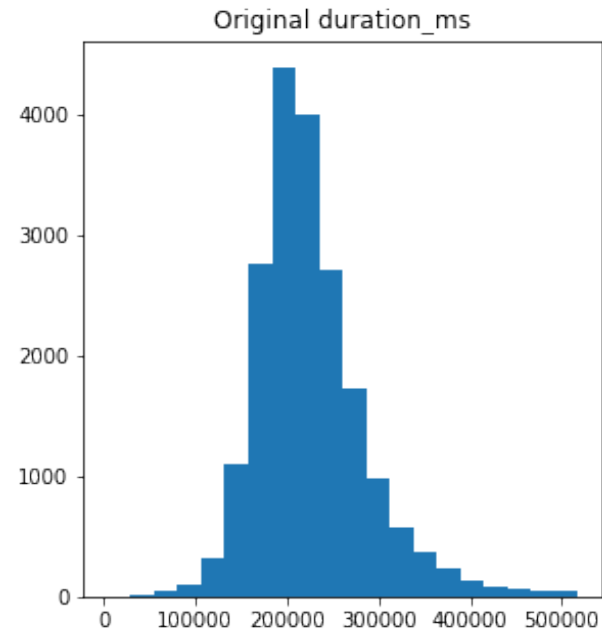
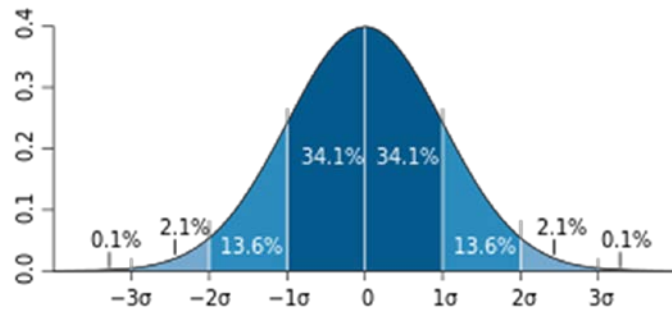


For hyper.parameter tuning, feature selection,  
model selection

## 2. Bring into consistent scale

**Standardization:**

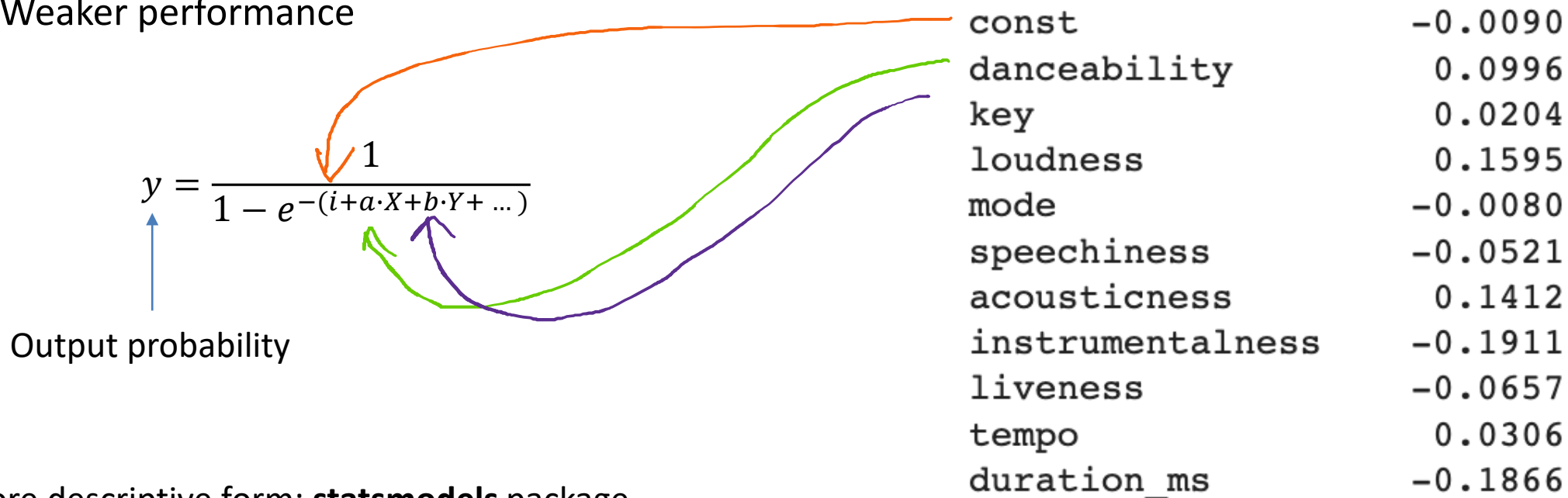
$$x_{std}^i = \frac{x^i - \mu_x}{\sigma_x}$$



Required by most ML/DL methods

## 3. Logistic regression

- Prefrectly explainable
- Easy implementation
- Weaker performance



More descriptive form: **statsmodels** package

## 4. Model performance metrics (classification)

**True positive (TP)** model predicts 1(popular song) and reality is 1(popular song)

**True negative (TN)** model predicts 0(less popular) and reality is 0(less popular)

**False positive (FP)** model predicts 1 and reality is 0

**False negative (FN)** model predicts 0 and reality is 1

- Default metric in **sklearn** : Accuracy =  $\frac{TP+TN}{TP+TN+FP+FN}$

- If the output is **not balanced**, F1 score should be used:

$$F1 = \frac{2 \cdot TP}{2 \cdot TP + FP + FN}$$

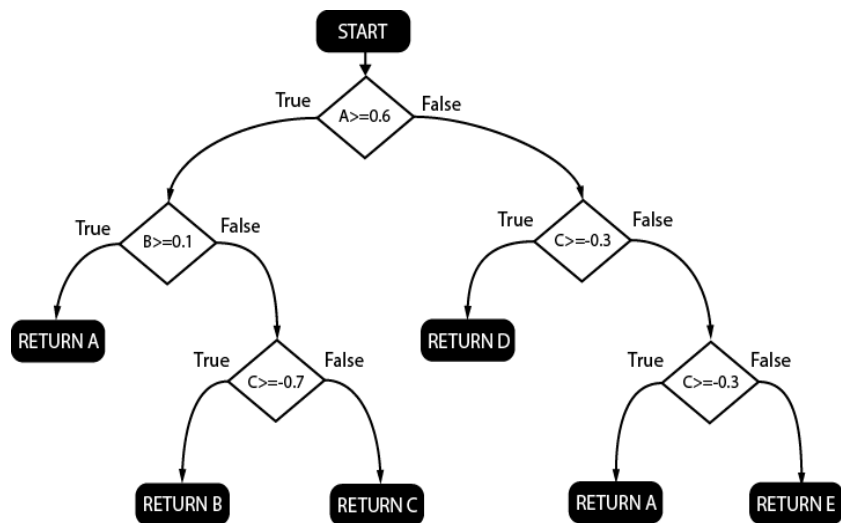
Example of an inbalanced dataset:  
100 patients, 10 ill, 90 healthy  
Classifier says „everybody is healthy“

TP	TN	FP	FN	Acc	F1
0	90	0	10	<b>0.9</b>	0.0

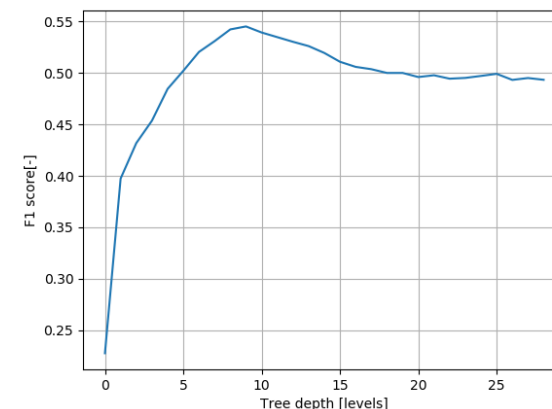
Perfect summarization table: <https://en.wikipedia.org/wiki/F-score>

## 5. Decision tree

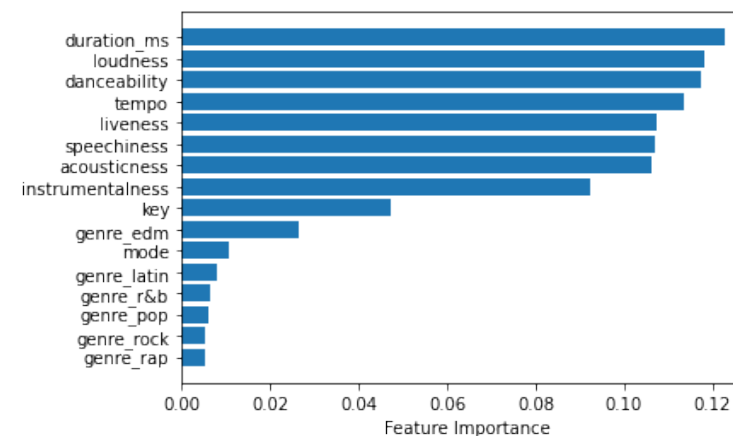
- Explainable
- Easy implementation. Does not care about scale/distribution
- Weaker performance. Easy to overfit



Decision tree example, classification into 6 classes



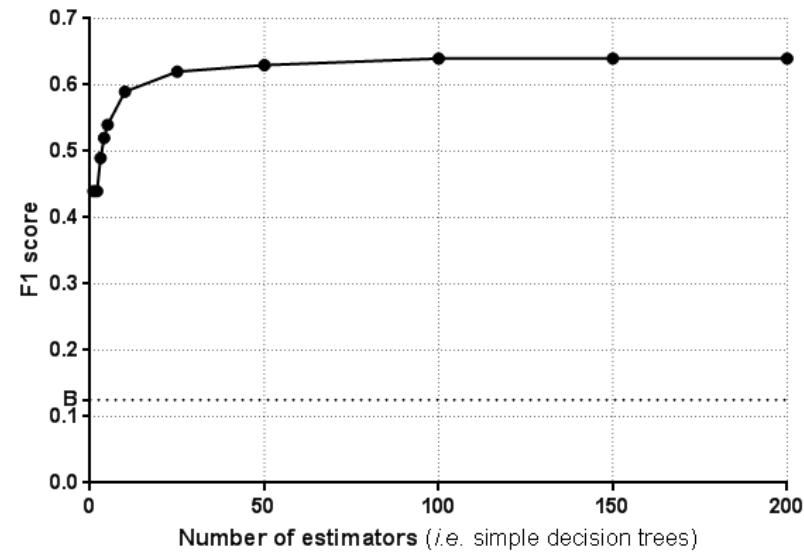
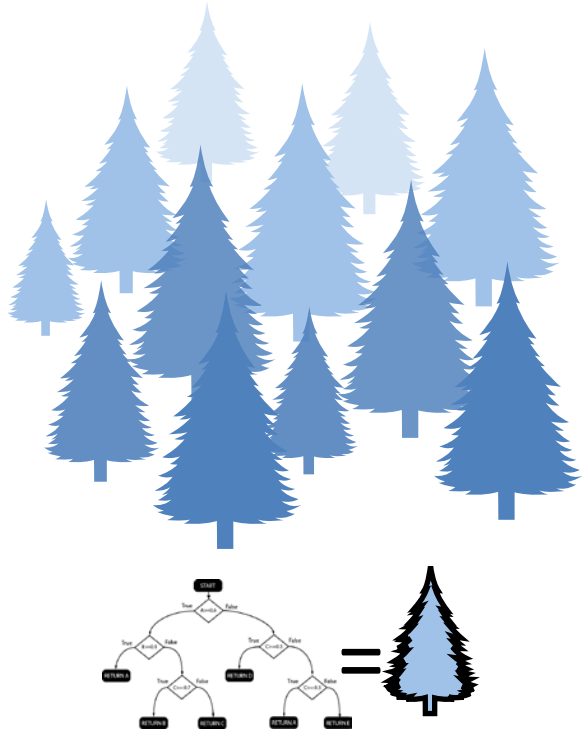
Performance by complexity



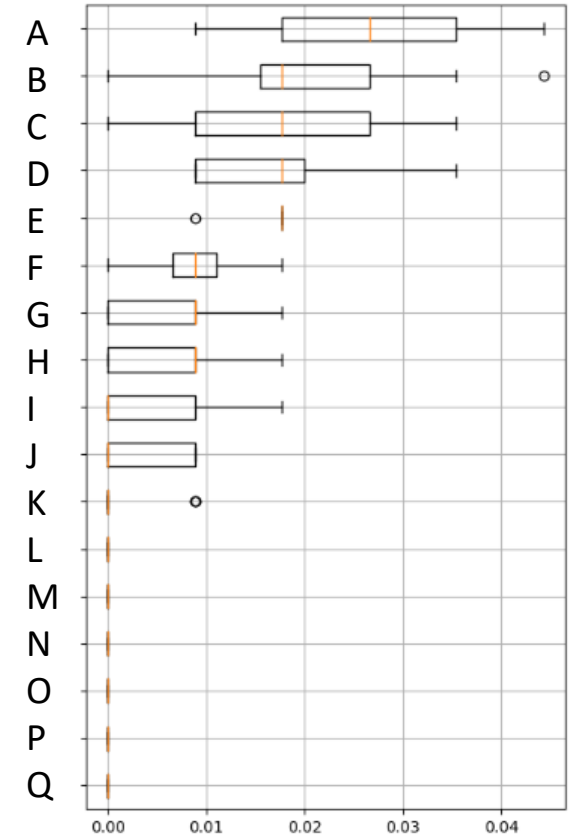
Feature importances in our MUSIC classification task

## 6. Random forest

- Still explainable (feature importance only)
- Does not care about ... anything



Forest performance by number of trees

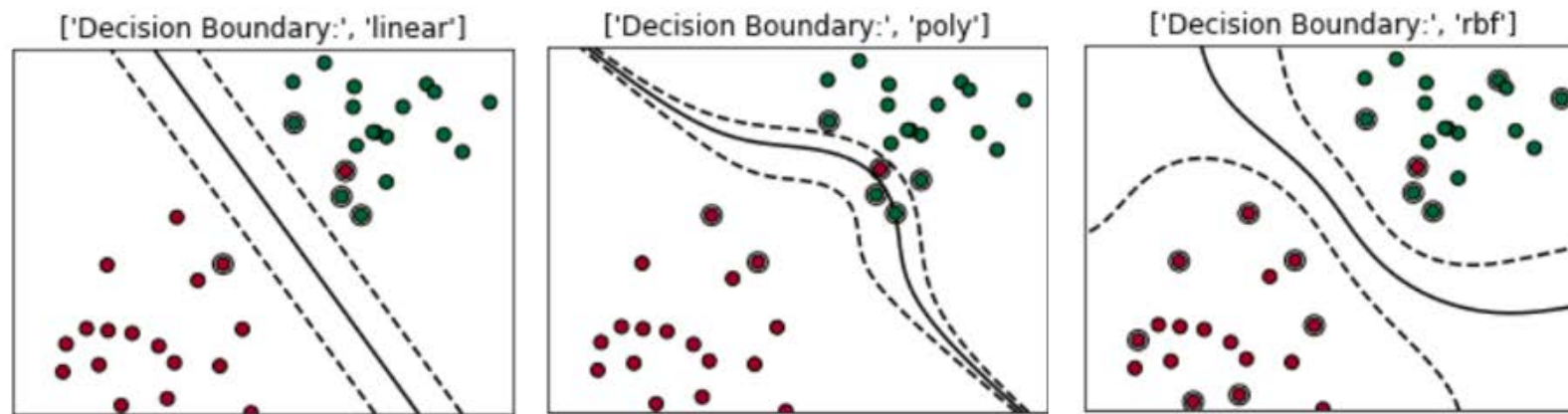


Permutation performance

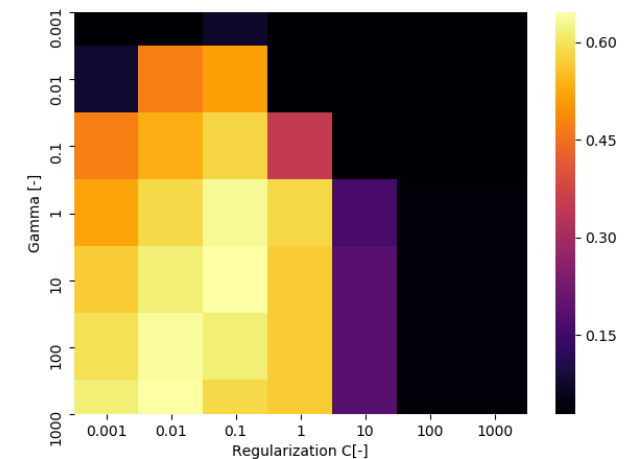


## 7. Support-vector-machines (SVM)

- Can use different „kernels“ – linear/polynomial/**radial-basis-function** (RBF) = default
- Stronger performance, but longer training time (the worst from class. ML methods)
- SVMs benefits from hyperparameter optimization



Source: <https://towardsdatascience.com/support-vector-machine-simply-explained-fee28eba5496>

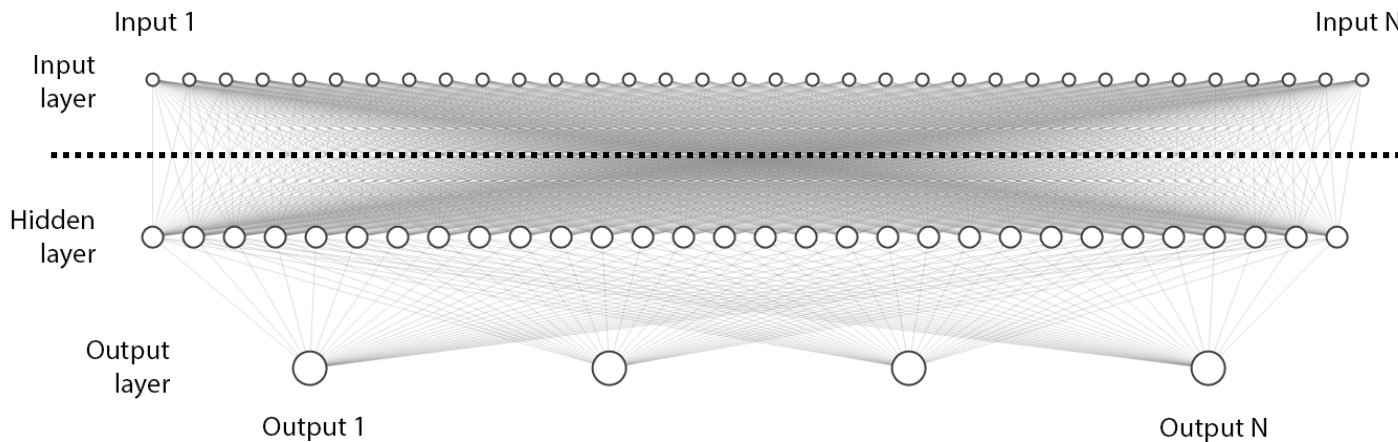


Performance by hyperparameters  
Gamma & regularization (def. 1)

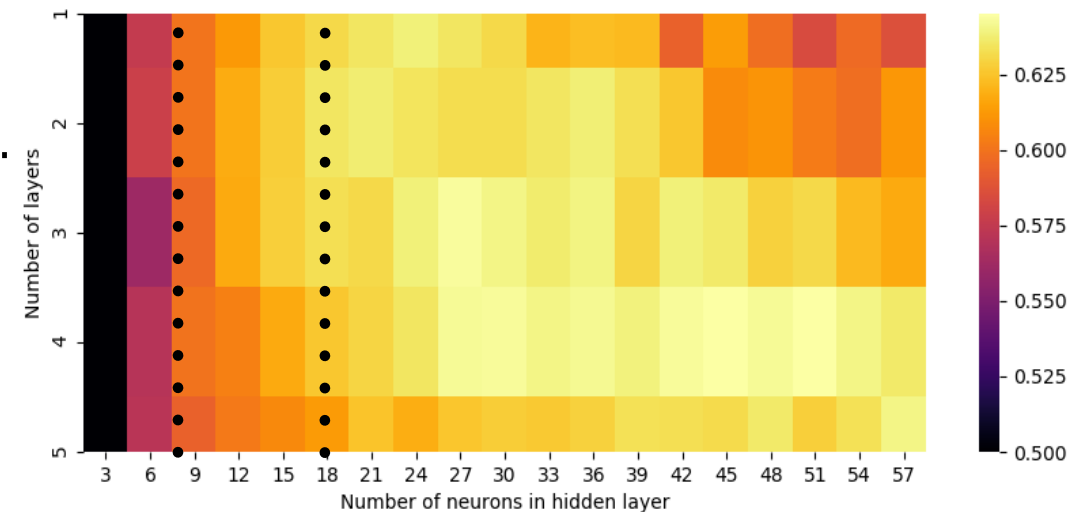
SVM usage in Epilepsy research: tomorrow 11:20 by B. Chybovski

## 8. Neural network (simple)

- Stronger performance (but usually do not performs better than RF or SVM-RBF)
- Needs „hyperparameter care“, trains longer than other ML methods
- They usually form **final building block of DL networks** (i.e. fully connected layer)



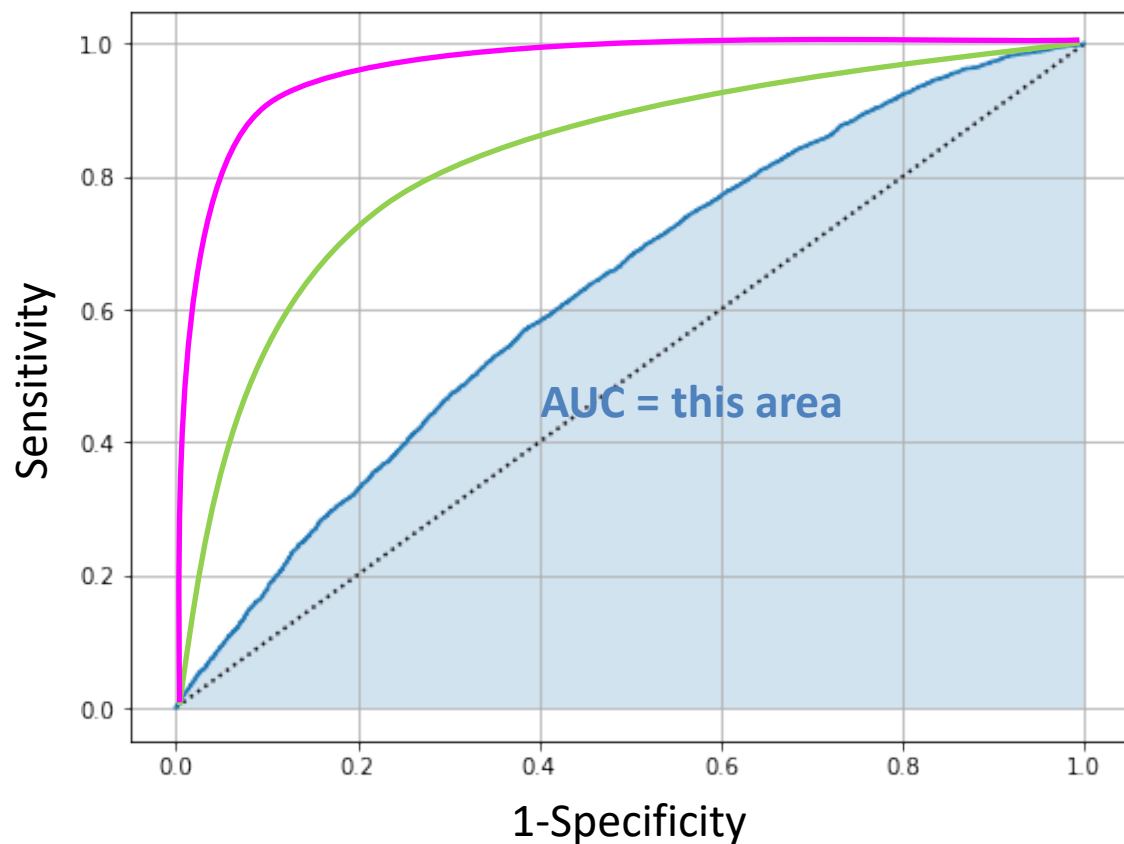
A typical shallow neural network



Performance (color) by neuron count in each hidden layer and by hidden layer count

## 9. Comparing models with AUC

- Area under ROC curve (ROC=Receiver-operating-characteristic)



$$\text{TPR} = \text{Sensitivity} = \frac{TP}{TP+FN}$$

$$\text{FPR} = 1 - \text{Specificity} = 1 - \frac{TN}{TN+FP}$$

- ..... 0.50 – useless classifier
- 0.63 – better classifier
- 0.80 – much better classifier
- 0.90 – wonderful classifier
- 1.00 – ultimate classifier
- <0.50 – probably mismatched labels

## 10. Summarization

- Incorrect (or none) data split to train/validation/test => incorrect predictive model
- Understanding data behavior is important for **model selection**
- Understanding **the target application** is important for **model selection**
- Different model types require specific data treatment (i.e., careful **feature selection** for LR models)
- It is practical to **standardize** data (but tree-based approaches do not need it)
- Models usually benefit from **hyperparameter tuning** (NNs, SVMs, simple trees)
- **More complex** model **does not necessarily mean** a **better** model performance
- Feature **explainability** depends on model type
- For building mentioned models, you need only the **sklearn** package

# Thank you for your attention

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Do you have any questions?

## Our further activities:

5.10.2022 – ICRC Academy (15:00, [here](#))

Umělá inteligence pro analýzu poruch srdeční činnosti

<https://akademie.fnusa.cz/?p=1311>

8.11.2022 – SignalPlant workshop (the whole day, [here](#))

signal analysis and processing

[www.signalplant.org](http://www.signalplant.org)

