Applied Machine Learning for Business Analytics

Lecture 8: Modeling

Lecturer: Zhao Rui

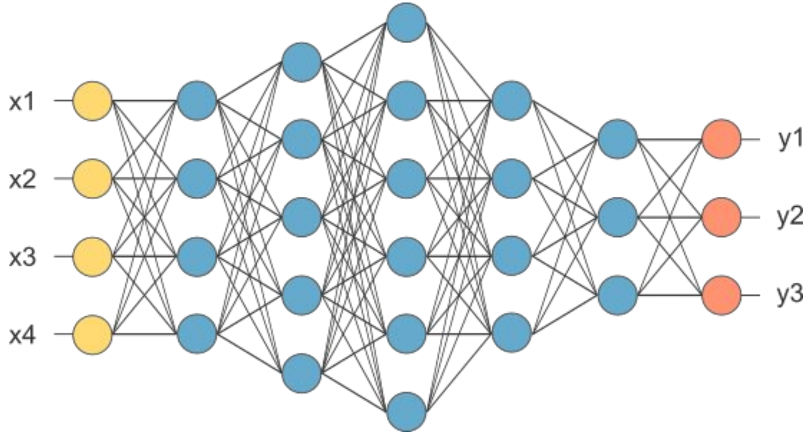
Agenda

1. Understanding Concepts behind ML Models
2. Ensembles
3. Explainable Machine Learning
4. Do not sleep on traditional machine learning

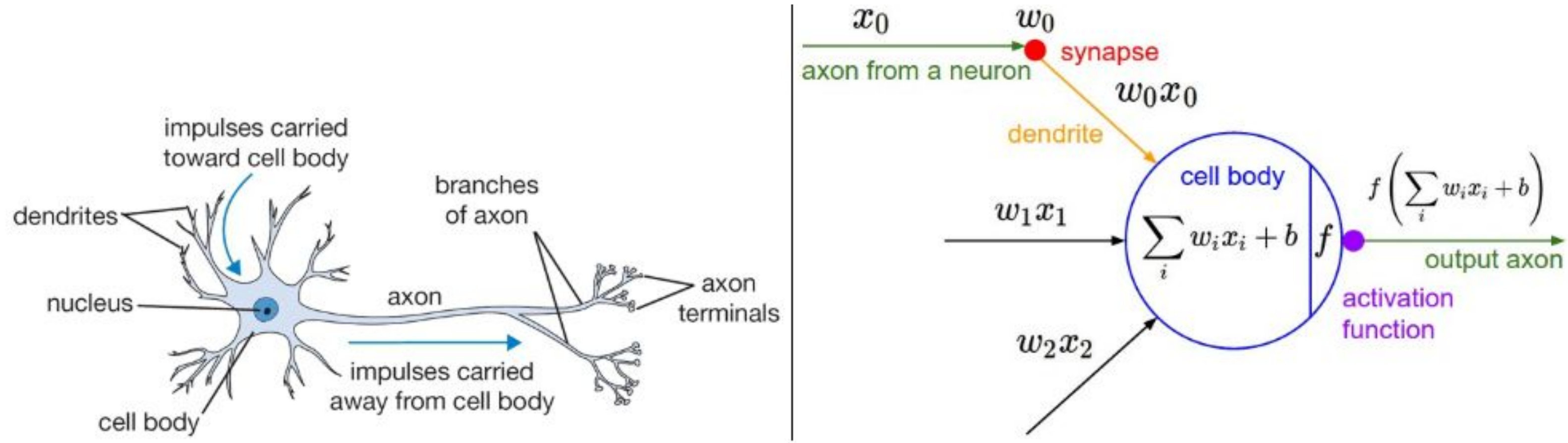
1. Understanding concepts

Take Neural network as an example

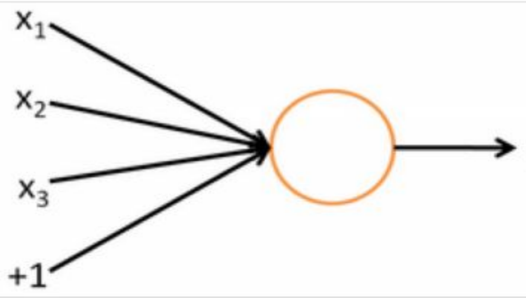
- From Wiki:
  - NN is based on a collection of connected units of nodes called artificial neurons which loosely model the neurons in a biological brain.
- From another way:
  - NN is running several ‘logistic regression’ at the same time (expanding at width and depth dimensions).



Neural computation



A cartoon drawing of a biological neuron (left) and its mathematical model (right).

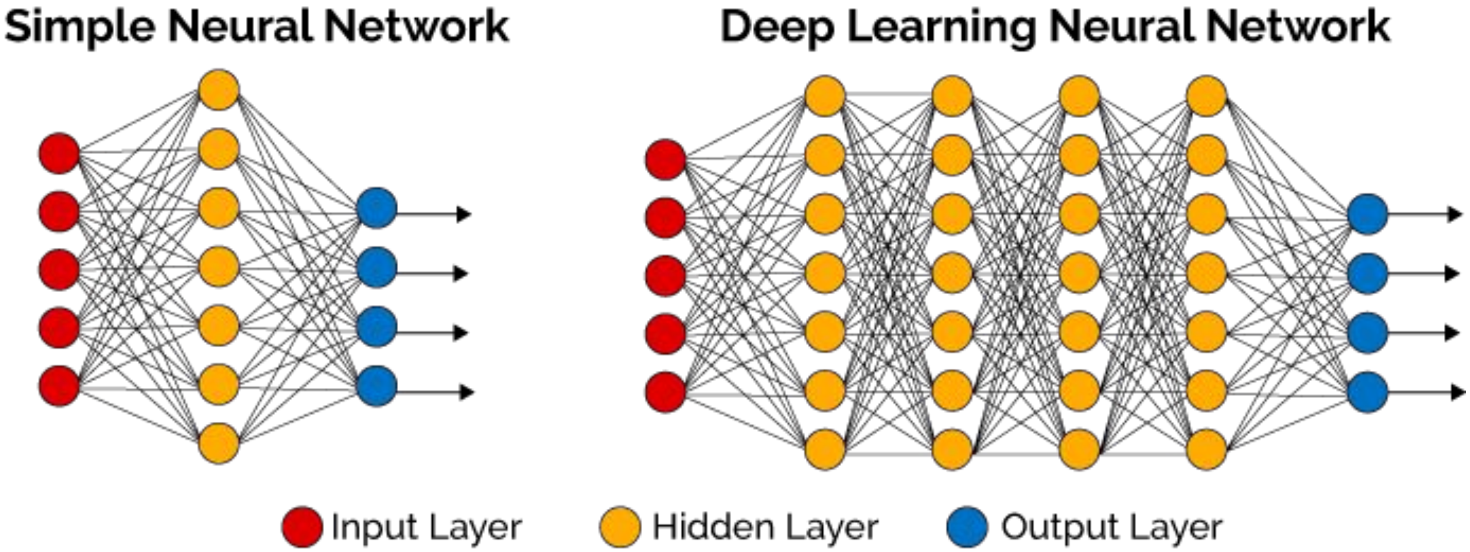


The fact that a neuron is essentially a logistic regression unit:

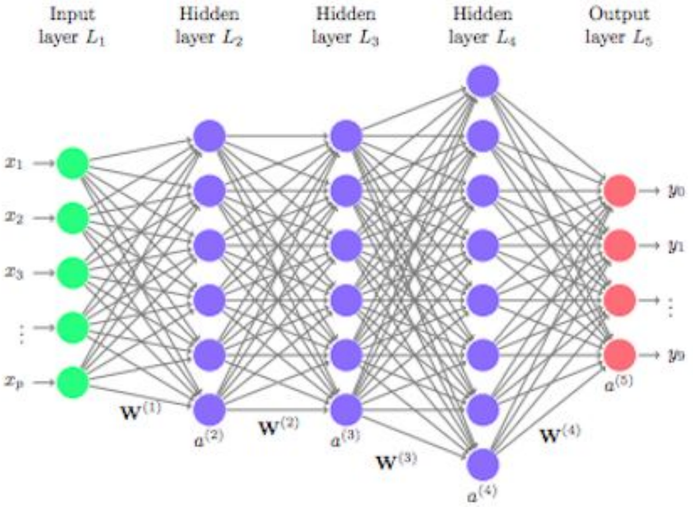
1 performs a dot product with the input and its weights

2 adds the bias and apply the non-linearity

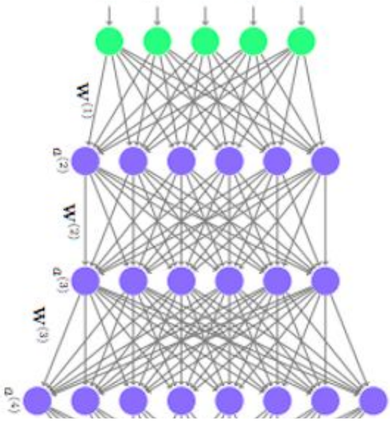
Shallow vs Deep



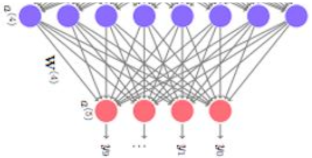
Hidden representation in deep learning



Low-dim, Original Space



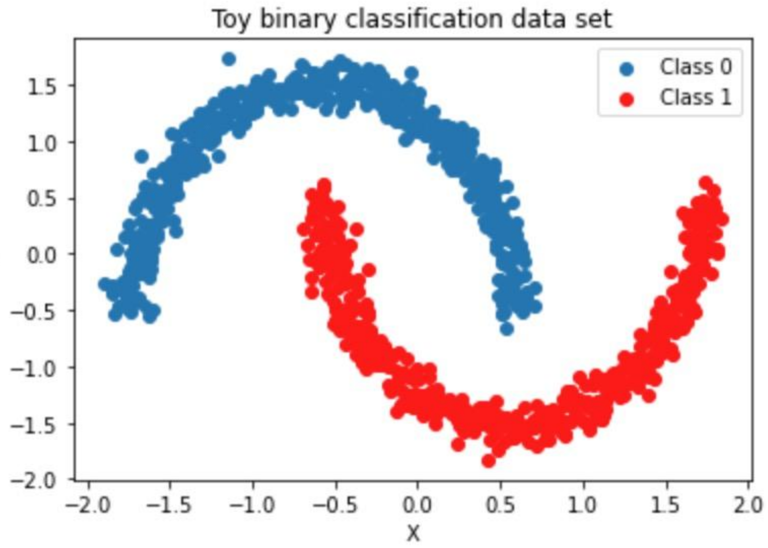
High-dim, **Linearly Separated** Space



Softmax Classifier
(Linear Model)

We want to project the data into the new feature/vector space that data is linearly separated

Moons Dataset




```python
# fit a logistic regression model to classify this data set as a benchmark
simple_model = LogisticRegression()
simple_model.fit(X_train, Y_train)
print('Train accuracy:', simple_model.score(X_train, Y_train))
print('Test accuracy:', simple_model.score(X_test, Y_test))
```

```
Train accuracy: 0.89
Test accuracy: 0.88
```

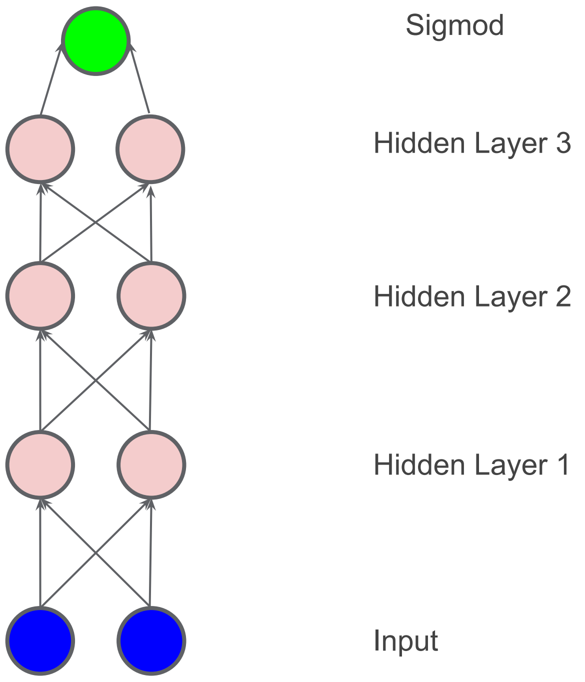
Fully-Connected Neural Network

```
# fix a width that is suited for visualizing the output of hidden layers
H = 2
input_dim = X.shape[1]

# create sequential multi-layer perceptron
model = Sequential()

# Then, use add() to insert layers into the container
model.add(Input(shape=(input_dim,)))
model.add(Dense(H,activation='tanh'))
model.add(Dense(H, activation='tanh'))
model.add(Dense(H, activation='tanh'))
#binary classification, one output
model.add(Dense(1, activation='sigmoid'))

model.compile(loss='binary_crossentropy',
              metrics=['acc'])
```



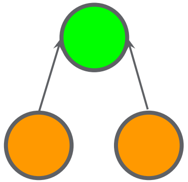
Fully-Connected Neural Network

```
# evaluate the training and testing performance of your model
# note: you should extract check both the loss function and your evaluation metric
score = model.evaluate(X_train, Y_train, verbose=0)
print('Train loss:', score[0])
print('Train accuracy:', score[1])
```

```
Train loss: 0.0007340409210883081
Train accuracy: 1.0
```

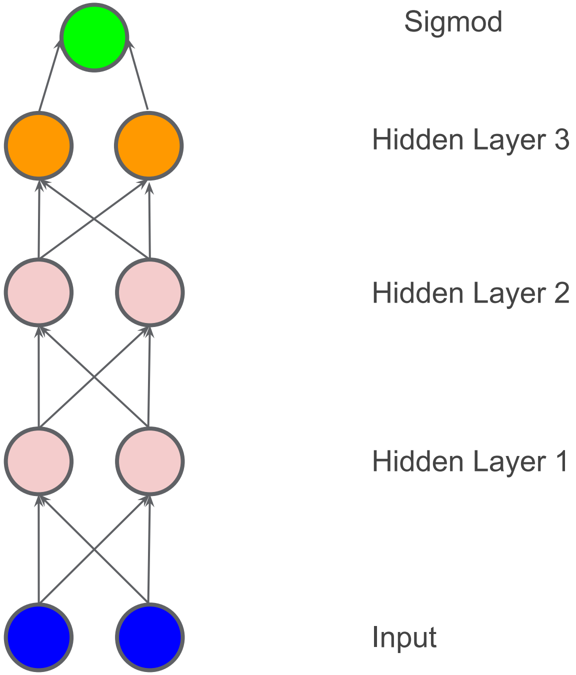
```
score = model.evaluate(X_test, Y_test, verbose=0)
print('Test loss:', score[0])
print('Test accuracy:', score[1])
```

```
Test loss: 0.0008793871384114027
Test accuracy: 1.0
```

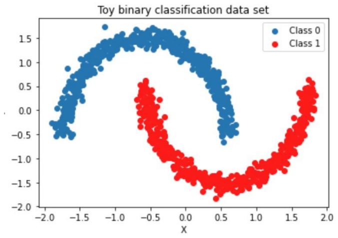


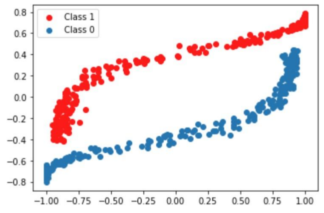
1. In forward computation, the output of hidden layer 3 is feed into “logistic regression” to predict labels.
2. Since the train and test accuracy are both 1, it means the hidden layer 3’ output are linearly separated.

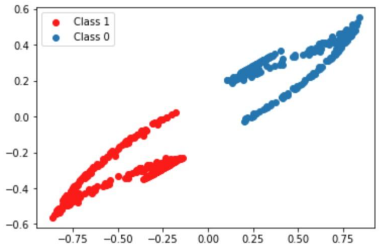
Let us visualize those outputs!

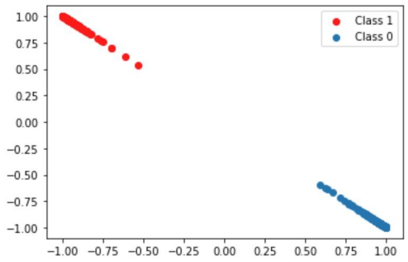


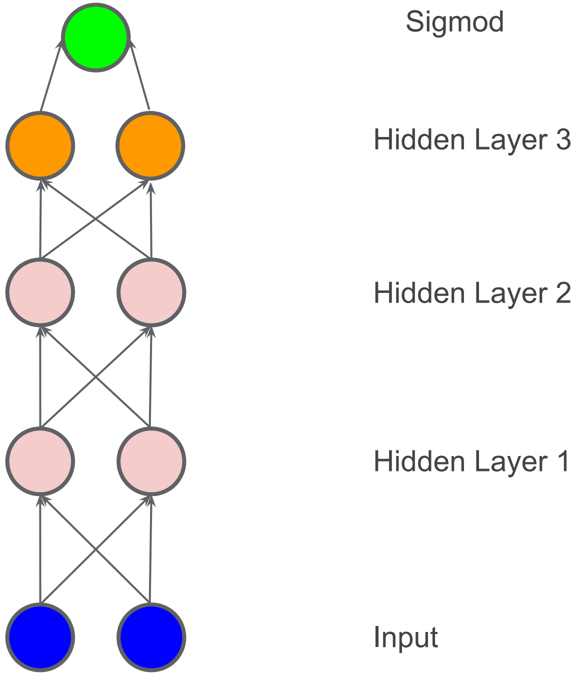
Fully-Connected Neural Network







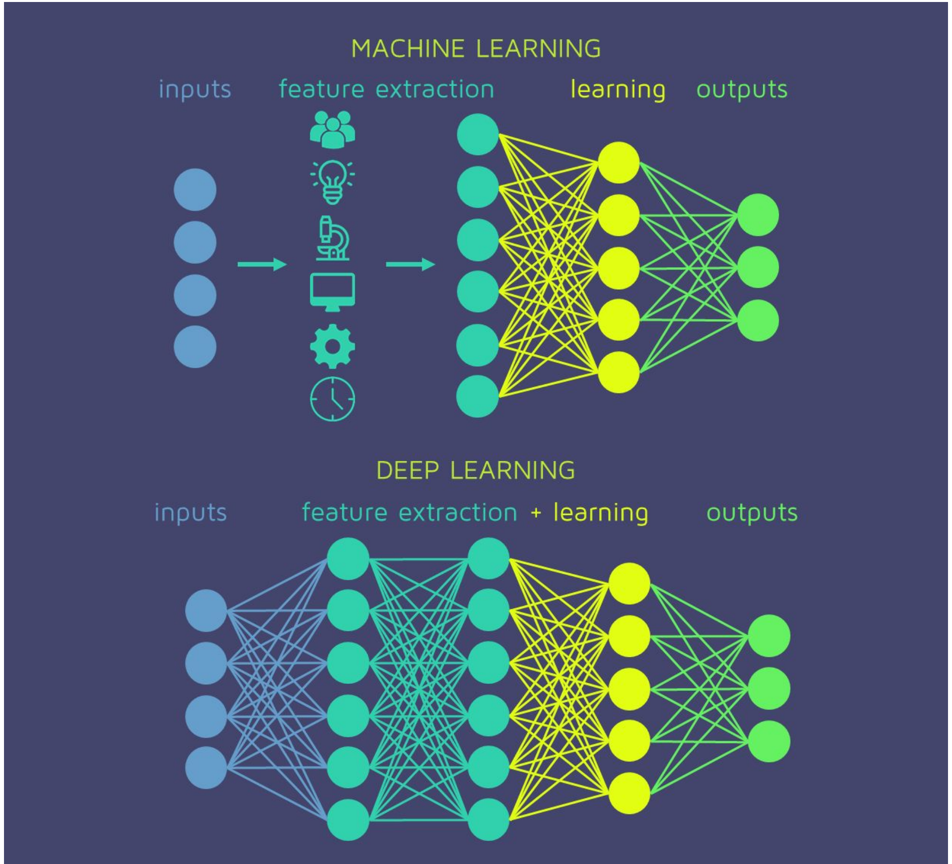




Representation Learning

https://github.com/rz0718/BT5153_2024/blob/main/codes/lab_lecture04/Representation_Learning.ipynb

End-to-end learning



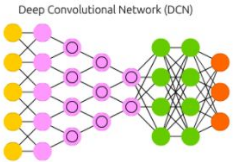
From Aporras

Representation Learning in Neural Networks

- Outputs of each hidden layer of an neural network is a non-linear transformation of the input data into a feature space. Each hidden layer should transform the input so that it is more linearly separable
- we are more interested in learning the latent representation of the data rather than perfecting our performance in a single task (such as classification).
    - We do not need to preprocess the data to add non-linear features. The neural network will learn the most suitable non-linear transformations to the input (to achieve the best classification)

Deep learning structures

CNNs

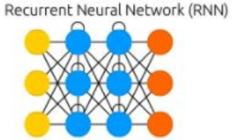


Local information

Weights sharing across steps

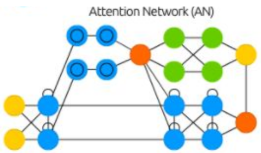
Fully-connected NNs

RNNs



Self-attention

Transformers



https://www.asimovinstitute.org/author/fjodorvanveen/

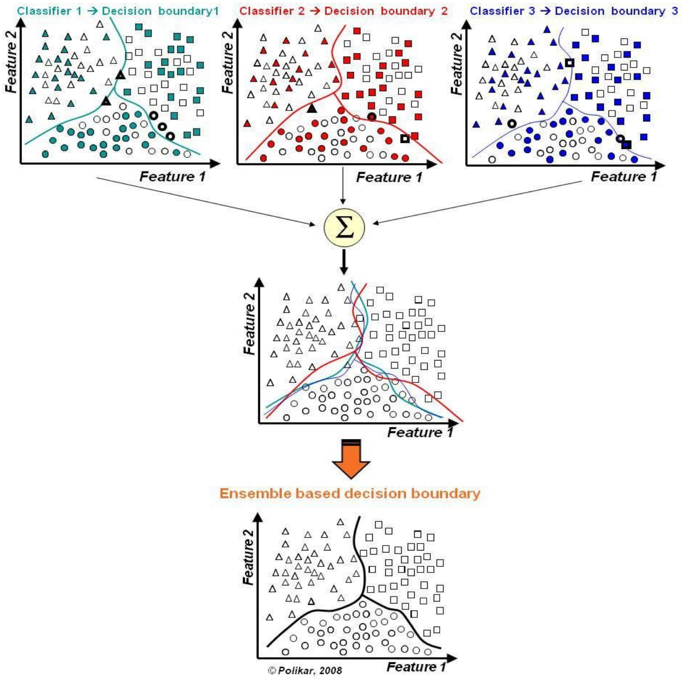
Understand your model’s assumption

- Independent and Identically Distributed-IID
  - **Neural networks** assume that examples are **independent and identically distributed**
- Smoothness
  - **Supervised algorithms** assume that there’s a set of functions that can transform inputs into outputs such that **similar inputs are transformed into similar outputs**
- Tractability
  - Let X be the input and Z be the latent representation of X. **Generative models** assume that it’s tractable to compute P(Z|X).
- Boundaries
  - **Linear classifiers** assume that **decision boundaries are linear**.
- Conditional independence
  - **Naive Bayes classifiers** assume that the **attribute values are independent of each other given the class.**

2. Ensemble

Ensemble

- Creating a strong model from an ensemble of weak models (base learners)



Ensembles: wining leaderboard (Kaggle & SOTA)

Leaderboard

SQuAD2.0 tests the ability of a system to not only answer reading comprehension questions, but also abstain when presented with a question that cannot be answered based on the provided paragraph.

Rank	Model	EM	F1
	Human Performance *Stanford University* (Rajpurkar & Jia et al. '18)	86.831	89.452
1 Sep 18, 2019	ALBERT (ensemble model) *Google Research & TTIC* https://arxiv.org/abs/1909.11942	**89.731**	**92.215**
2 Jul 22, 2019	XLNet + DAAF + Verifier (ensemble) *PINGAN Omni-Sinitic*	88.592	90.859
2 Sep 16, 2019	ALBERT (single model) *Google Research & TTIC* https://arxiv.org/abs/1909.11942	88.107	90.902
2 Jul 26, 2019	UPM (ensemble) *Anonymous*	88.231	90.713
3 Aug 04, 2019	XLNet + SG-Net Verifier (ensemble) *Shanghai Jiao Tong University & CloudWalk* https://arxiv.org/abs/1908.05147	88.174	90.702

1st PLACE - WINNER SOLUTION - Gilberto Titericz & Stanislav Semenov

1st PLACE SOLUTION - Gilberto Titericz & Stanislav Semenov

First, thanks to Organizers and Kaggle for such great competition.

Our solution is based in a 3-layer learning architecture as shown in the picture attached.

-1st level: there are about 33 models that we used their predictions as meta features for the 2nd level, also there are 8 engineered features.

https://www.kaggle.com/c/otto-group-product-classification-challenge/discussion/14335

Why does ensembling work

- Task: credit card fraud detection (Normal/Fraudulent)
- 3 **uncorrelated** models, each with accuracy of 80%
- Ensemble: Majority voting
    - When at least two models are correct, ensemble model would be correct

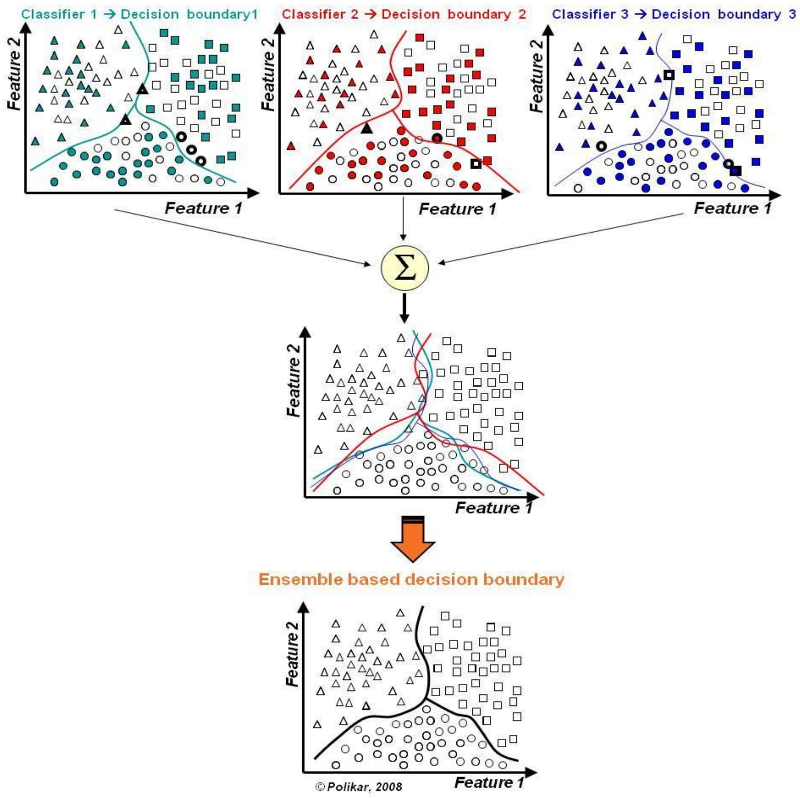
Why does ensembling work

- Ensemble Accuracy:
  - Probability that at least two models are correct:

Outputs of 3 models	Probability	Ensemble’s output
All 3 are correct	0.8 * 0.8 * 0.8 = 0.512	Correct
Only 2 are correct	(0.8 * 0.8 * 0.2) * 3 = 0.384	Correct
Only 1 is correct	(0.2 * 0.2 * 0.8) * 3 = 0.096	Wrong
None is correct	0.2 * 0.2 * 0.2 = 0.008	Wrong

Why does ensembling work

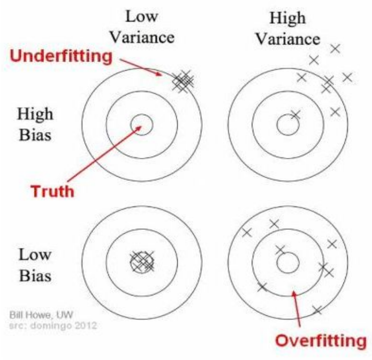
- Reduce Bias
- Reduce Variance



Prediction Error = Bias ^ 2 + Variance + Irreducible Error

Bias-Variance

- Bias:
  - The difference between the average prediction of our model and the correct value which we are trying to predict
- Variance:
  - The variability of model prediction for a given data point or a value which tells us spread of data



Reduce Bias

- Assume a test set of 10 samples and k (assume k is odd) **uncorrelated** binary classifiers, where each classifier has ***p*** accuracy
- The accuracy of ensembling using majority voting
  - The probability that majority of classifiers are correct

$$\sum_{i=0}^{int(\frac{k}{2})} \binom{k}{i} p^{k-i}(1-p)^{i}$$

What is the probability that k choose ***i classifiers*** whose predictions are **wrong** and the rest ***k-i models***' outputs are **correct**.

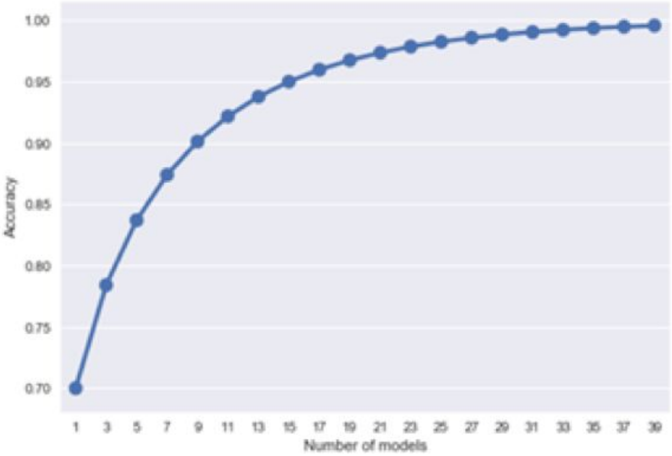
Reduce Bias

- Change the number of models

$$\sum_{i=0}^{\lfloor \frac{k}{2} \rfloor} \binom{k}{i} p^{k-i} (1-p)^i$$

If p = 0.7, then we have

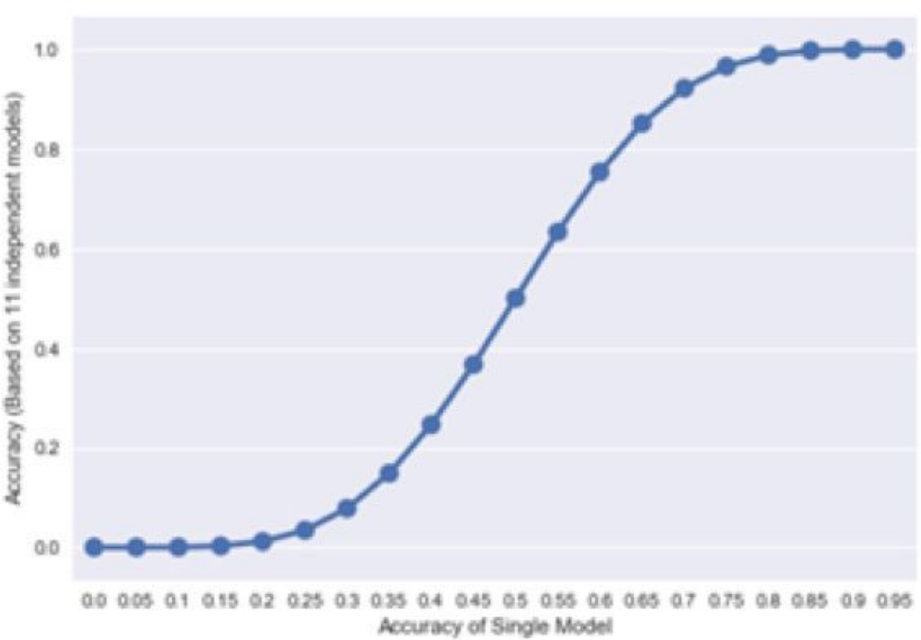
k	Ensemble Accuracy
1	0.7
3	0.784
5	0.83692
11	0.92177520904
101	0.999987057446



Reduce Bias

- Change the accuracy of the base model $\sum_{i=0}^{\lfloor \frac{k}{2} \rfloor} \binom{k}{i} p^{k-i} (1-p)^i$

Fix # of classifiers to be 11



Reduce Variance

- Suppose we have n **independent** models: M1, M2, ..., Mn with the same variance $\boldsymbol{\sigma}$ **^2**
- The ensemble M* constructed from those models using averaging will have the variance as follows:

$$
\begin{aligned}
Var(M^*) &= Var(\frac{1}{n}\sum_i M_i) \\
&= \frac{1}{n^2} Var(\sum_i M_i) \\
&= \frac{1}{n^2} * n * Var(M_i) \\
&= \frac{Var(M_i)}{n}
\end{aligned}
$$

$$\sigma^2 \rightarrow \frac{\sigma^2}{n}$$

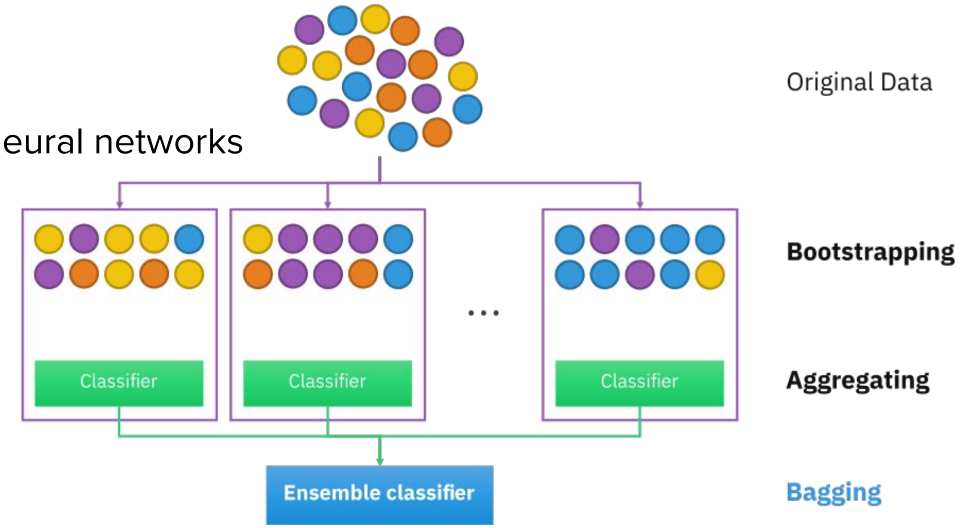
Ensemble

- Bagging: reduce the variance in the model
    - Random Forest
- Boosting: reduce the bias in a model
    - Ada-Boost, XGBoost
- Stacking: increase the prediction accuracy of a model
    - [MLxtend]()

- **The less correlation among base learners, the better**
- **Try to have different model architectures for base learners**

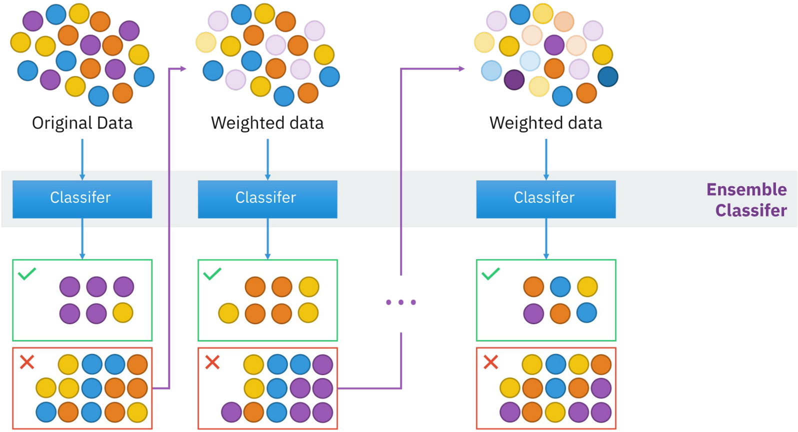
Bagging

- Sample with replacement to create different datasets
- Train a classifier with each dataset
- Aggregate predictions from classifiers
  - Majority Voting:
    - Equal and weighted combinations
- Decreases errors by decreasing the variance
- Can improve unstable methods such as trees, neural networks



Boosting

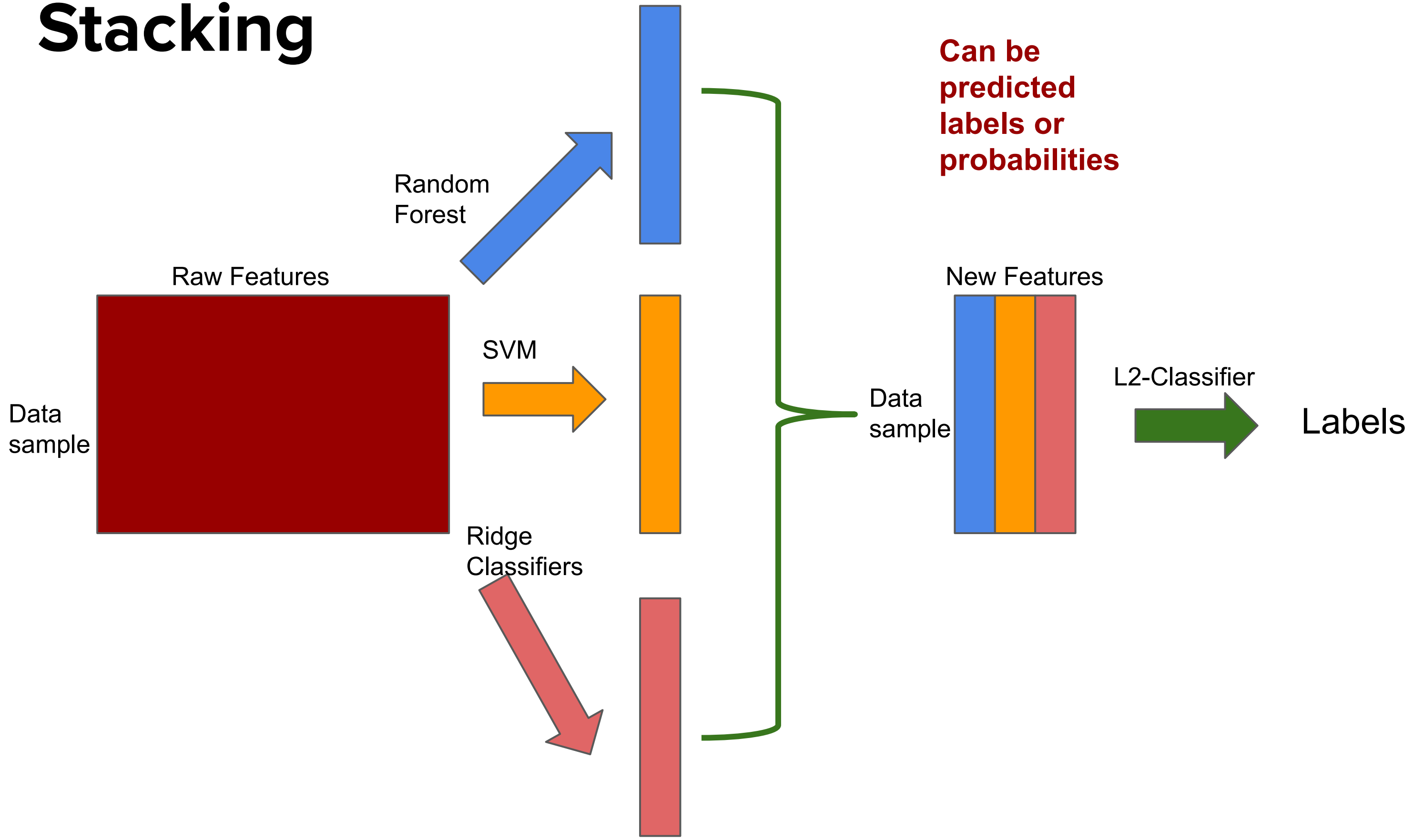
- Train a weak classifier
- Give samples misclassified by weak classifier higher weight
- Repeat (1) on this reweighted data as many iterations as needed
- Final strong classifier: weighted combination of existing classifiers
    - classifiers with smaller training errors have higher weights
- Popular methods for tabular data:
    - Gradient Boosting
    - AdaBoost
    - XGBoost
    - LigtGBM



Stacking

- Core idea: use a pool of base classifiers, then using another classifier (stacker) to combine their prediction for the final decision

Stacking


Can be predicted labels or probabilities
Random Forest
Raw Features
SVM
Data sample
Ridge Classifiers
New Features
Data sample
L2-Classifier
Labels

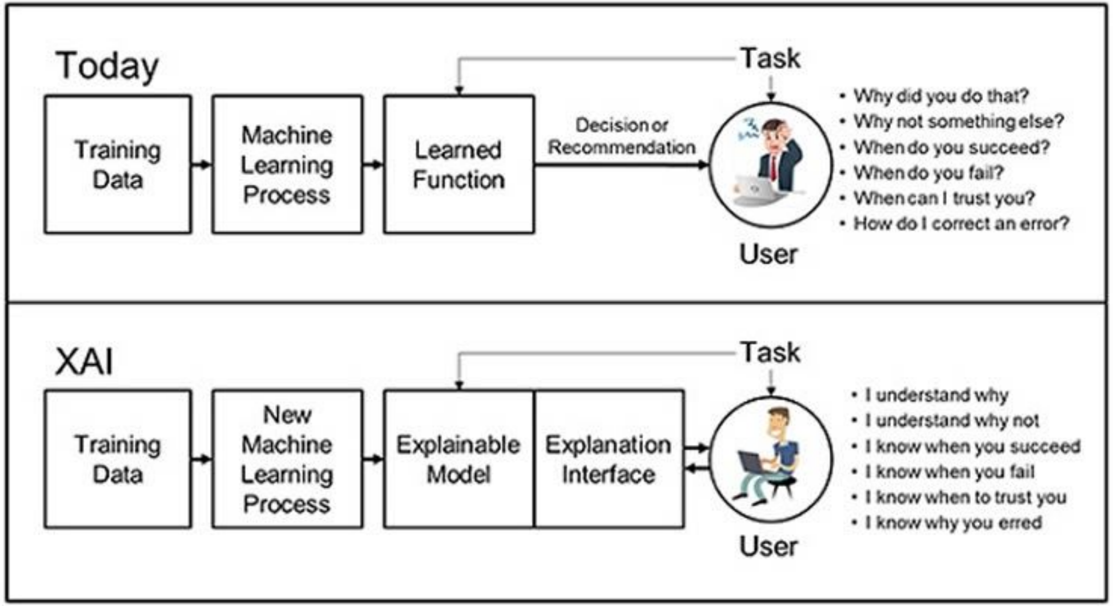
Some possible pitfalls of Ensemble

- Exponentially increasing training times and computational requirements
- Increase demand on infra. To maintain and update these models
- Greater chance of data leakage between models or stages in the whole training

3. Explainable Machine Learning

Explainable AI (XAI)

- **XAI**: ML models are explainable that enable end users to understand, appropriately trust, and effectively manage the emerging generation for AI systems.



DARPA's report

Linear Models First

- Prediction is the linear combinations of the features values, weighted by the model coefficients.

Students A’s chance = 0.2 + 0.1* GPA - 0.005 * Hours on Tiktok

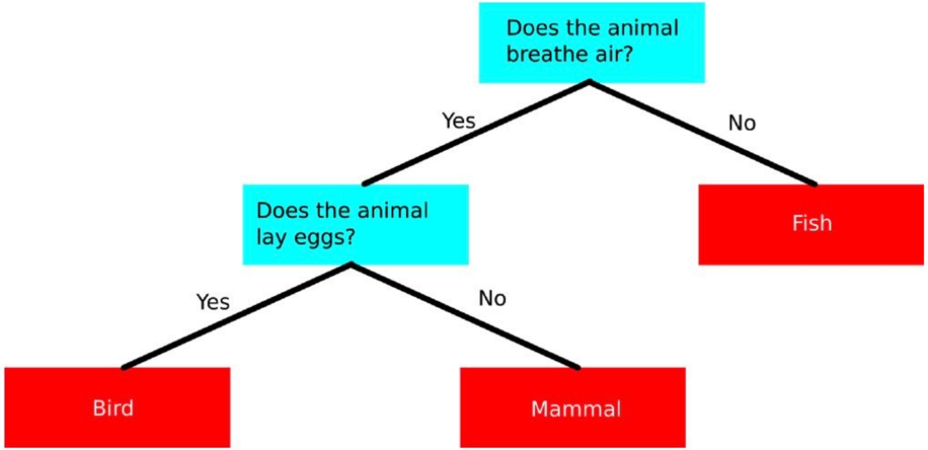
One student’s feature
GPA: 5
Hours on Tiktok: 60 hours

Feature Contributions
GPA: 0.5
Hours on Tiktok: -0.3

- Capability of linear models is limited.

Decision Tree

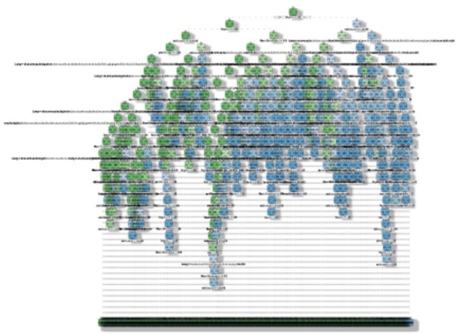
- It is “interpretable”
- More powerful compared to linear models.



Source:
https://towardsdatascience.com/a-beginners-guide-to-decision-tree-classification-6d3209353ea

Decision Tree can be complex

It can be a huge and complex tree.

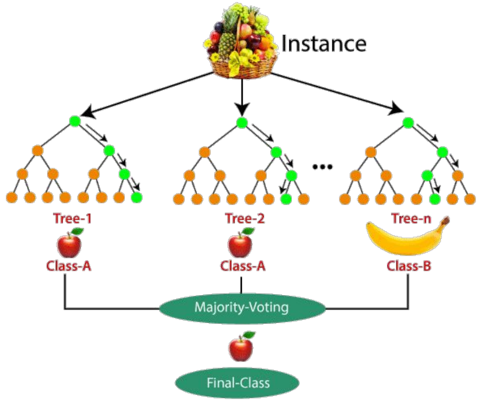


Rattle 2016-Aug-18 16:15:42 sklisarov

My goal is to extract some useful rules from the entire process to implement in a score card.

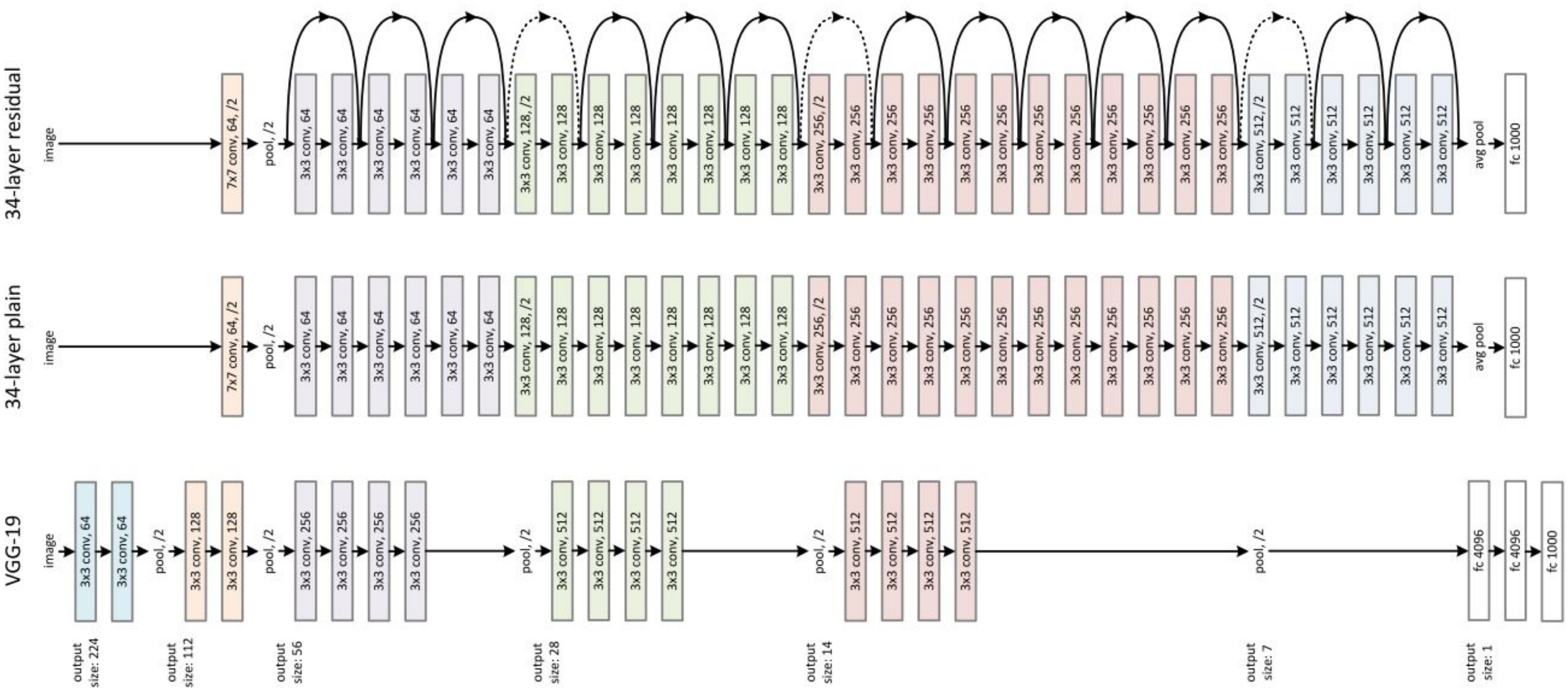
https://stats.stackexchange.com/questions/230581/decision-tree-too-large-to-interpret

It can be a forest



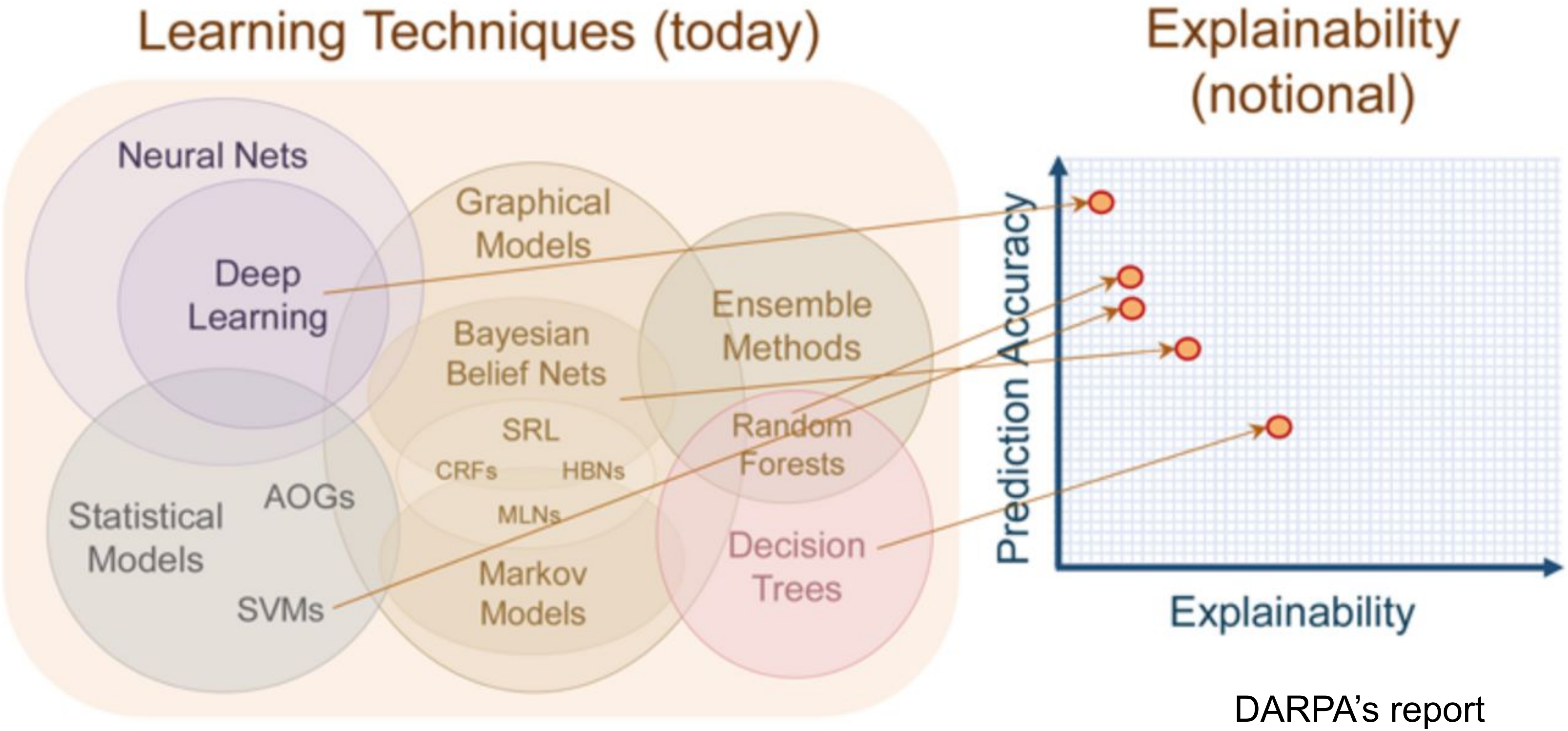
https://www.javatpoint.com/machine-learning-random-forest-algorithm

Complex Models



For imagenet, they use 152 layers, which firstly achieved lower error rate compared to Humans in image recognition tasks.

Trade-off



DARPA's report

Pokemon vs Digimon

https://medium.com/@DataStevenson/teaching-a-computer-to-classify-anime-8c77bc89b881

Task Definition

Training Data

Digimon

Pokemon

Testing Data

Digimon or Pokemon?

Task Definition

```
from keras.models import Sequential
from keras.layers import Conv2D, MaxPooling2D
from keras.layers import Activation, Dropout, Flatten, Dense

model = Sequential()
model.add(Conv2D(32, (3, 3), input_shape=(150, 150, 3)))
model.add(Activation('relu'))
model.add(MaxPooling2D(pool_size=(2, 2)))
model.add(Flatten())  # this converts our 3D feature maps to 1D feature vectors
model.add(Dense(64))
model.add(Activation('relu'))
model.add(Dropout(0.5))
model.add(Dense(1, activation='sigmoid', name='preds'))

model.compile(loss='binary_crossentropy',
              optimizer='rmsprop',
              metrics=['accuracy'])
```

```
Epoch 1/3
8/8 [==============================] - 12s 2s/step - loss: 2.7443 - accuracy: 0.7675 - val_
loss: 0.0834 - val_accuracy: 0.9922
Epoch 2/3
8/8 [==============================] - 12s 2s/step - loss: 0.0560 - accuracy: 0.9835 - val_
loss: 0.0692 - val_accuracy: 0.9961
Epoch 3/3
8/8 [==============================] - 12s 1s/step - loss: 0.0559 - accuracy: 0.9856 - val_
loss: 0.0684 - val_accuracy: 0.9961
```

The implementation and dataset could be found on this week notebook

Only after three epochs, the testing/val accuracy was easily over 99%. Amazing!

Gradient-based Method

- Explain the decision made by the model
  - Eg, Why do you think this image is pokemon not digimon?

- Motivation: we want to know the contribution of each **component/feature** in the input data for prediction

Pixel, Segment in Images

Word in text

This is BT5153

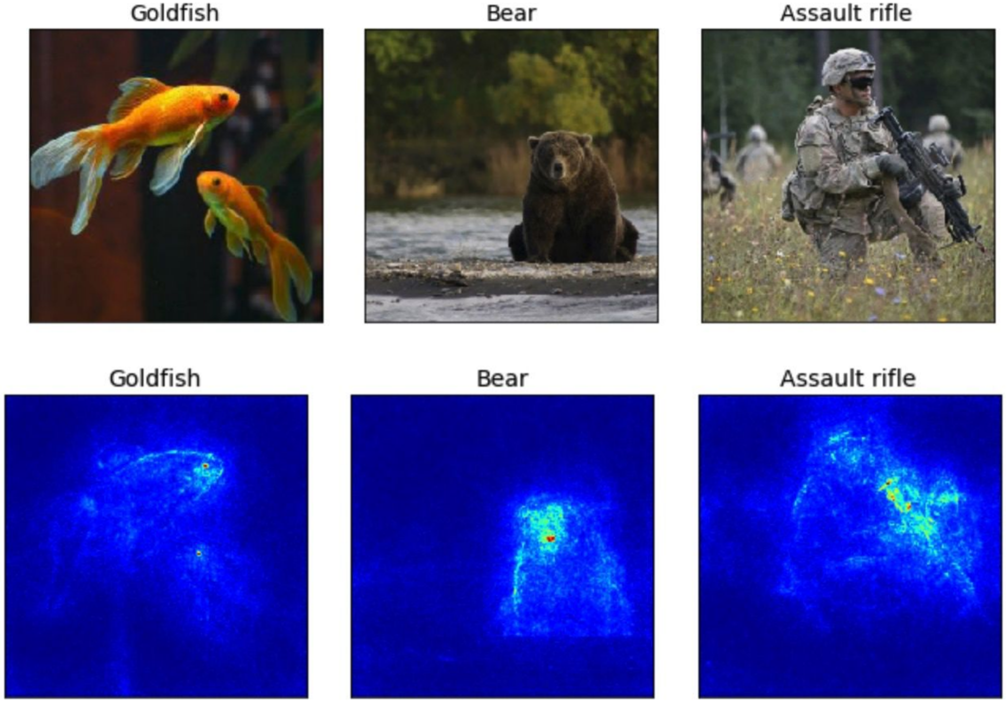
- Solution: Removing or modifying the partial parts of the components, observing the change of decision.

Saliency Map

$$\{x_1, \ldots, x_i, \ldots, x_n\} \qquad \{x_1, \ldots, x_i + \Delta x, \ldots, x_n\}$$

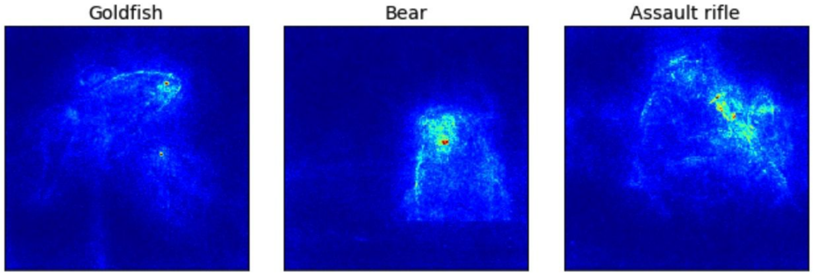
$$y_k \qquad y_k + \Delta y$$

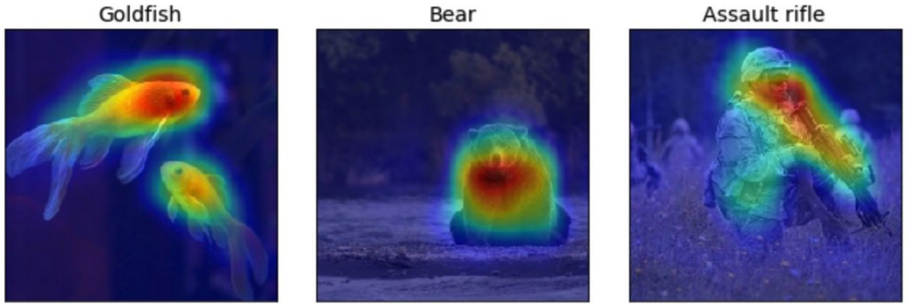
$$\left|\frac{\Delta y}{\Delta x}\right| \qquad \left|\frac{\partial y}{\partial x}\right|$$



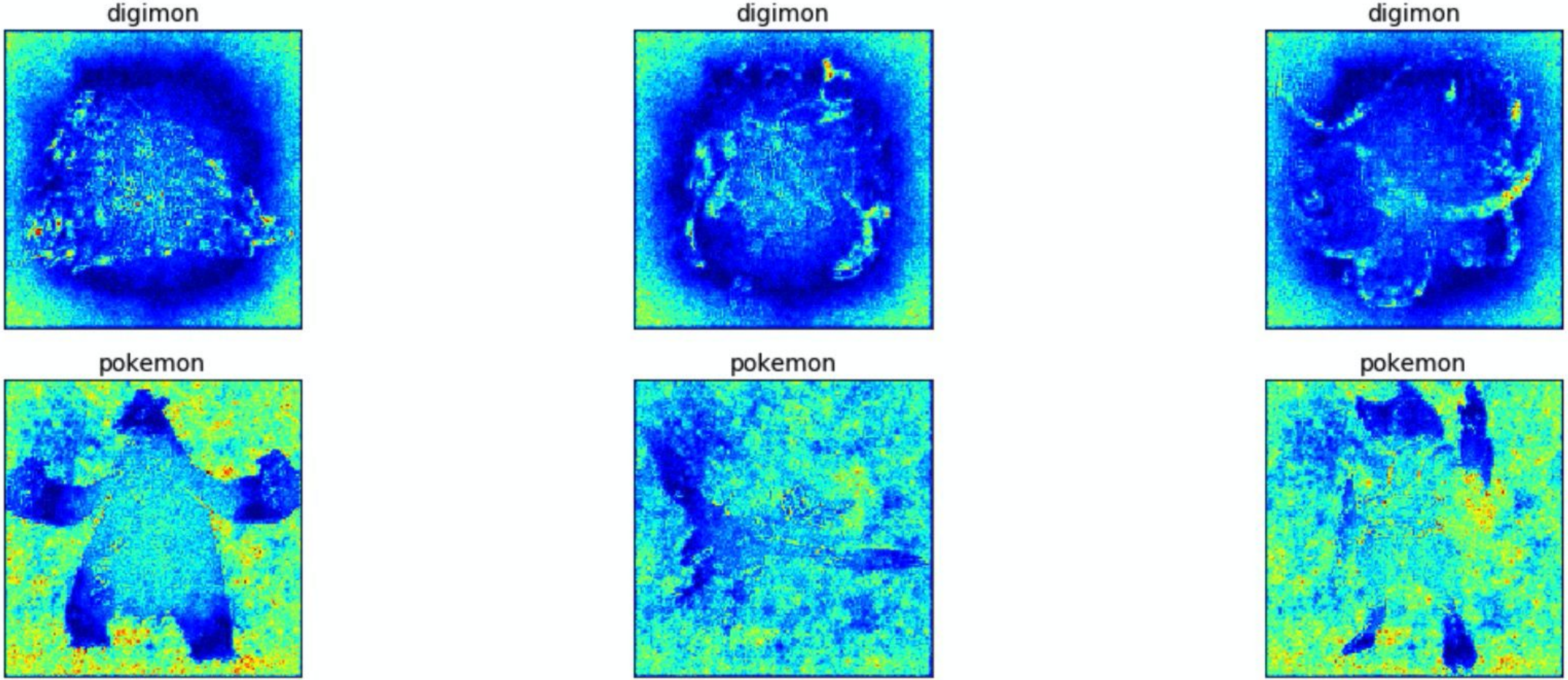
Andrea Vedaldi, Andrew Zisserman, "Deep Inside Convolutional Networks: Visualising Image Classification Models and Saliency Maps", ICLR, 2014

Saliency Map

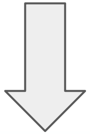




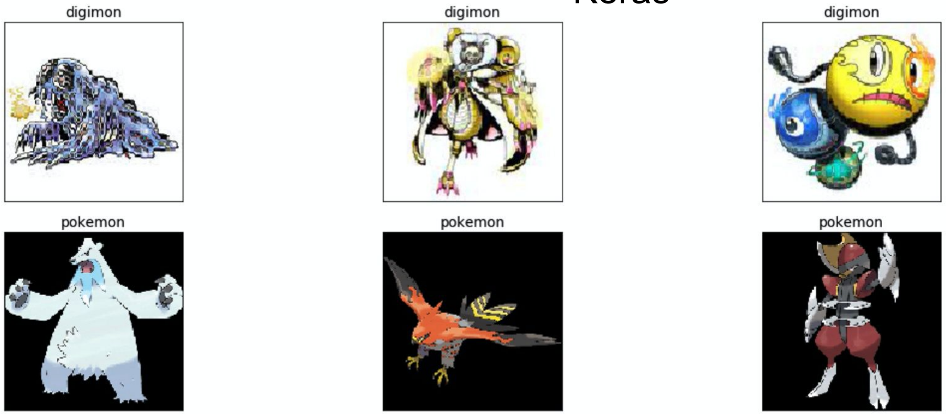
Pokemon vs Digimon



Pokemon vs Digimon



Loaded by Keras



CNN only learns to classify pokemon and digimon based on background colors.

PNG all appear in full black background

https://stackoverflow.com/questions/55720576/keras-loaded-png-appears-full-black

4. Do not sleep on traditional machine learning

Why do tree-based models still outperform deep learning on tabular data?

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Abstract

Model comparison

Tree-based Models outperform deep learning on tabular data

Based on 45 middle-sized datasets (10, 000 samples)

From this paper, authors explain:

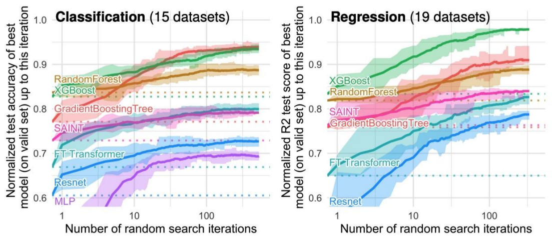

Figure 1: **Benchmark on medium-sized datasets, with only numerical features**. Dotted lines correspond to the score of the default hyperparameters, which is also the first random search iteration. Each value corresponds to the test score of the best model (on the validation set) after a specific number of random search iterations, averaged on 15 shuffles of the random search order. The ribbon corresponds to the minimum and maximum scores on these 15 shuffles.

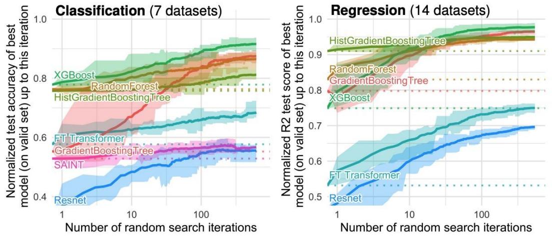

Figure 2: **Benchmark on medium-sized datasets, with both numerical and categorical features**. Dotted lines correspond to the score of the default hyperparameters, which is also the first random search iteration. Each value corresponds to the test score of the best model (on the validation set) after a specific number of random search iterations, averaged on 15 shuffles of the random search order. The ribbon corresponds to the minimum and maximum scores on these 15 shuffles.

- Deep learning bias to the overly smooth solution, while tree-based models are able to generate irregular decision boundaries
- Deep learning are very sensitive to uninformative features which could be easily spotted in tabular data, while tree-based models are more robust

Deep Learning for time series data

- “Results show that competitive performance can be achieved with a conventional machine learning pipeline consisting of **preprocessing**, **feature extraction**, and a **simple machine learning model**. In particular, we analyze the performance of a linear model and a non-linear (gradient boosting) model”

Table 3
Comparison between the proposed classical machine learning pipeline and other (deep learning) solutions using macro F1-score (MF1), overall accuracy (ACC), and Cohen’s Kappa coefficient (κ). The approaches are sorted according to macro F1. The scores in bold represent the best score for each dataset (that are comparable to our approach).

Dataset	Year	System	Technique	LP	MF1	ACC	κ	Signals
Sleep-EDF-SC-20	2021	RobustSleepNet [28]	RNN	FT	0,817	–	–	EEG + EOG
	2022	*This work*	Catboost	DT	**0,810**	**0,866**	**0,816**	EEG + EOG + EMG
	2021	XSleepnet2 [46]	CNN & RNN	LFS	0,809	0,864	0,813	EEG + EOG
	2022	*This work*	Logistic regr.	LFS	0,809	0,857	0,806	EEG + EOG + EMG
	2022	*This work*	Logistic regr.	DT	0,805	0,863	0,813	EEG + EOG + EMG
	2020	TinySleepNet [47]	CNN & RNN	LFS	0,805	0,854	0,800	EEG
	2020	SimpleSleepNet [48]	RNN	LFS	0,805	–	–	EEG + EOG
	2022	*This work*	Logistic regr.	LFS	0,803	0,853	0,800	EEG + EOG
	2022	*This work*	Catboost	LFS	0,802	0,864	0,812	EEG + EOG + EMG
	2020	XSleepnet1 [46]	CNN & RNN	LFS	0,798	0,852	0,798	EEG + EOG
	2022	*This work*	Catboost	LFS	0,797	0,860	0,807	EEG + EOG
	2019	SleepEEGNet [44]	CNN & RNN	LFS	0,797	0,843	0,790	EEG
	2020	SeqSleepNet+ [45]	RNN	FT	0,796	0,852	0,789	EEG
	2021	RobustSleepNet [28]	RNN	LFS	0,791	–	–	EEG + EOG
	2021	RobustSleepNet [28]	RNN	DT	0,791	–	–	EEG + EOG
	2020	DeepSleepNet+ [45]	CNN	FT	0,790	0,846	0,782	EEG + EOG
	2021	DeepSleepNet-Lite [15]	CNN	LFS	0,780	0,840	0,780	EEG
	2019	IITNet [43]	CNN & RNN	LFS	0,776	0,839	0,780	EEG
	2017	DeepSleepNet [41]	CNN & RNN	FT	0,769	0,820	0,760	EEG
Sleep-EDF-SC-78	2022	SleepTransformer [40]	transformer	FT	0,788	0,849	0,789	EEG
	2021	XSleepnet2 [46]	CNN & RNN	LFS	**0,787**	**0,840**	**0,778**	EEG + EOG
	2020	XSleepnet1 [46]	CNN & RNN	LFS	0,784	0,840	0,777	EEG
	2020	TinySleepNet [47]	CNN & RNN	LFS	0,781	0,831	0,770	EEG
	2021	RobustSleepNet [28]	RNN	FT	0,779	–	–	EEG + EOG
	2022	*This work*	Catboost	LFS	0,775	0,831	0,766	EEG + EOG + EMG
	2022	*This work*	Catboost	LFS	0,772	0,830	0,763	EEG + EOG
	2022	*This work*	Logistic regr.	LFS	0,771	0,821	0,756	EEG + EOG + EMG
	2022	*This work*	Logistic regr.	LFS	0,768	0,820	0,753	EEG + EOG
	2021	RobustSleepNet [28]	RNN	LFS	0,763	–	–	EEG + EOG
	2021	DeepSleepNet-Lite [15]	CNN	LFS	0,752	0,803	0,730	EEG
	2022	SleepTransformer [40]	transformer	LFS	0,743	0,814	0,743	EEG
	2021	RobustSleepNet [28]	RNN	DT	0,738	–	–	EEG + EOG
	2019	SleepEEGNet [44]	CNN & RNN	LFS	0,736	0,800	0,730	EEG
Sleep-EDF-ST	2021	RobustSleepNet [28]	RNN	FT	0,810	–	–	EEG + EOG
	2022	*This work*	Catboost	LFS	**0,795**	**0,836**	**0,765**	EEG + EOG + EMG
	2022	*This work*	Logistic regr.	LFS	0,792	0,829	0,759	EEG + EOG + EMG
	2021	RobustSleepNet [28]	RNN	DT	0,791	–	–	EEG + EOG
	2022	*This work*	Catboost	LFS	0,789	0,832	0,758	EEG + EOG
	2022	*This work*	Logistic regr.	LFS	0,788	0,825	0,754	EEG + EOG
	2021	RobustSleepNet [28]	RNN	LFS	0,786	–	–	EEG + EOG
	2020	DeepSleepNet+ [45]	CNN	FT	0,775	0,815	0,738	EEG
	2020	SeqSleepNet+ [45]	RNN	FT	0,775	0,810	0,734	EEG
MASS SS3	2020	SimpleSleepNet [48]	RNN	LFS	**0,847**	–	–	EEG + EOG
	2021	RobustSleepNet [28]	RNN	FT	0,840	–	–	EEG + EOG
	2020	TinySleepNet [47]	CNN & RNN	LFS	0,832	**0,875**	**0,820**	EEG
	2021	RobustSleepNet [28]	RNN	LFS	0,822	–	–	EEG + EOG
	2022	*This work*	Catboost	LFS	0,817	0,867	0,803	EEG + EOG + EMG
	2017	DeepSleepNet [41]	CNN & RNN	FT	0,817	0,862	0,800	EEG
	2022	*This work*	Catboost	LFS	0,809	0,863	0,797	EEG + EOG
	2021	RobustSleepNet [28]	RNN	DT	0,808	–	–	EEG + EOG
	2022	*This work*	Logistic regr.	LFS	0,807	0,853	0,786	EEG + EOG + EMG
	2019	IITNet [43]	CNN & RNN	LFS	0,805	0,863	0,790	EEG
	2021	U-Sleep [29]	CNN	DT	0,800	–	–	EEG + EOG
	2022	*This work*	Logistic regr.	LFS	0,794	0,845	0,775	EEG + EOG

Do not sleep on traditional machine learning: Simple and interpretable techniques are competitive to deep learning for sleep scoring ☆

Jeroen Van Der Donckt [1], Jonas Van Der Donckt [1], Emiel Deprost, Nicolas Vandenbussche, Michael Rademaker, Gilles Vandewiele, Sofie Van Hoecke

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Source: https://www.sciencedirect.com/science/article/abs/pii/S1746809422008837

Deep Learning for unstructured data

- Deep learning are good at capturing high dimensional and spatial patterns/interactions among data
- Therefore, in those domains such as image, video, and text, deep learning is able to achieve huge success especially enough data are present

Next Class: Model Evaluation