



AutoML and Explainable AI

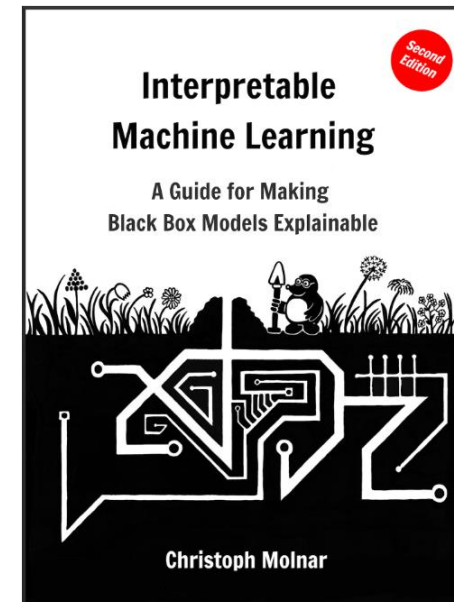
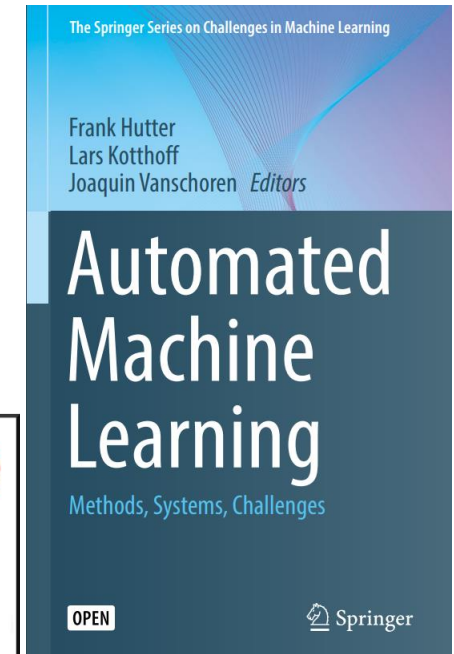
Assoc. Prof. Karl Ezra Pilario, Ph.D.

Process Systems Engineering Laboratory
Department of Chemical Engineering
University of the Philippines Diliman

Outline

- AutoML Packages
 - Lazy Predict
 - Auto-sklearn
 - Optuna
 - TPOT
- Explainable AI (XAI)
 - Definitions and Concepts
 - Permutation Feature Importance
 - Drop-column Feature Importance
 - Mean-Decrease-in-Impurity
 - Shapley Additive Explanations

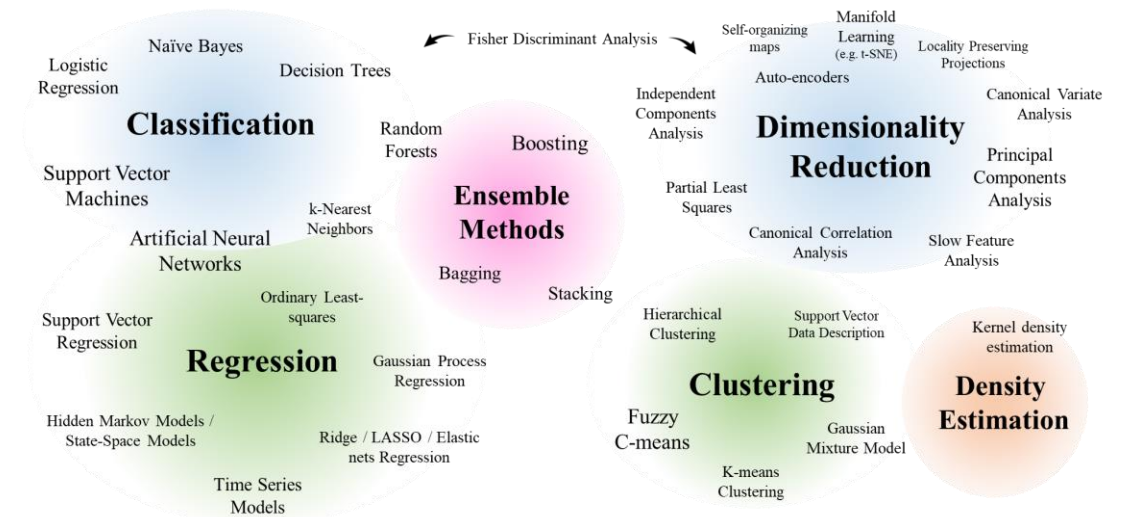
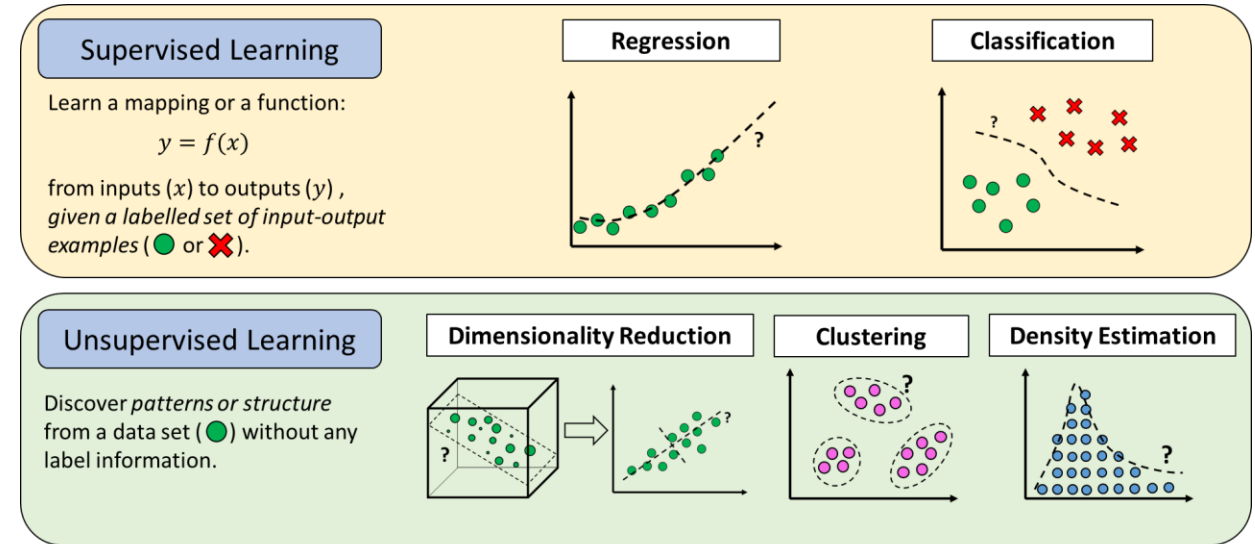
Hutter, Kotthoff,
Vanschoren (2019)



Molnar (2022)

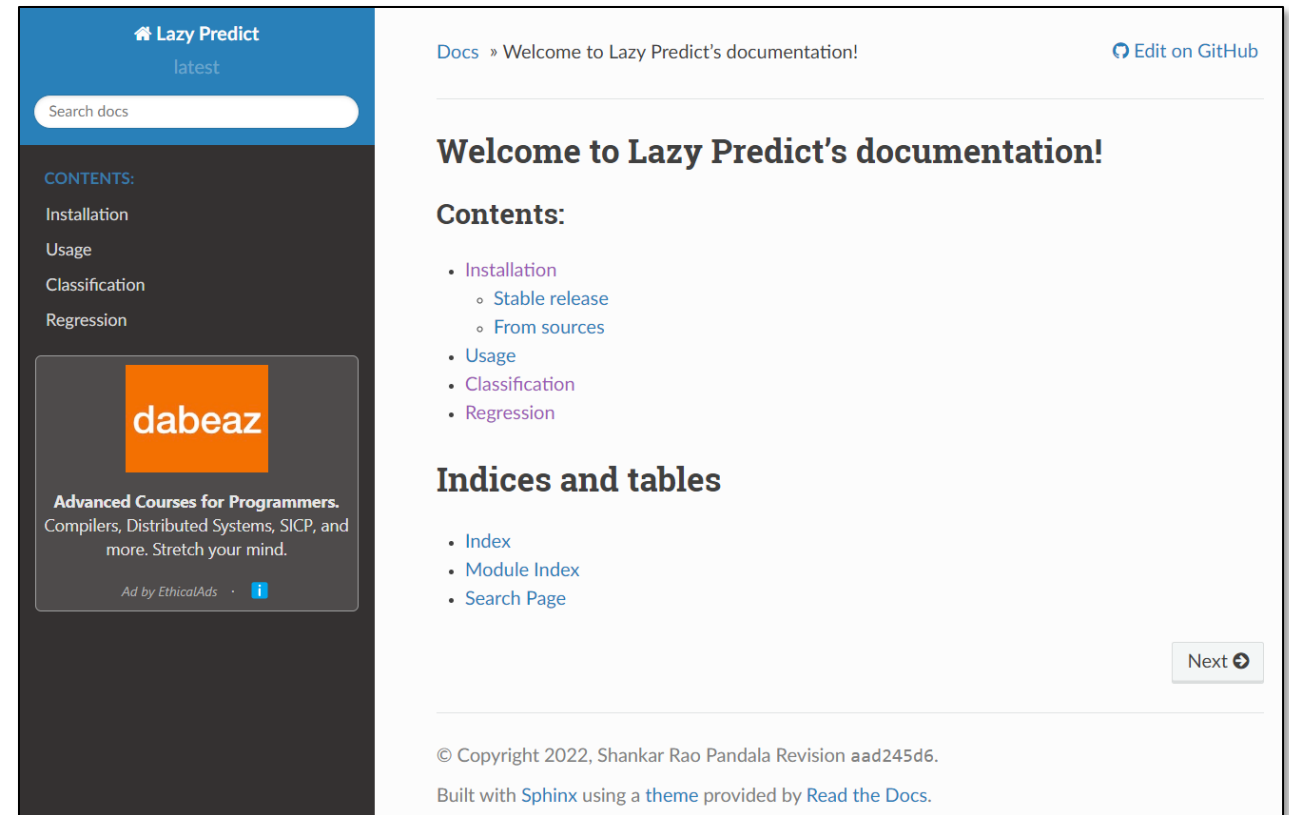
AutoML

- Automatically discover best-performing models with little user involvement.
- For model comparison, AutoML offers a single hyperparameter optimization toolkit for all models.
- Meta-learning: Learning to Learn**
 - The science of systematically observing how different ML approaches perform on a wide range of tasks, then learning from this experience to improve ML itself.
- CASH: Combined Algorithm Selection and Hyperparameter Optimization (Kotthoff et al., 2019)**
 - Automatically and simultaneously choosing a learning algorithm and setting its hyperparameters to optimize empirical performance.



Lazy Predict

- Shankar Rao Pandala (Last Update: 2022)
- <https://github.com/shankarpandala/lazypredict/tree/master>
- <https://lazypredict.readthedocs.io/en/latest/>
- Fits a number of **scikit-learn** models on the data with default settings for all.
- Results: Accuracy, R2, F1-score, etc.
- No automatic model selection nor hyper-parameter tuning.
- For classification or regression only.



The screenshot displays the documentation for 'Lazy Predict'. The left sidebar features a blue header with the project name and version, a search bar, and a 'CONTENTS' menu listing Installation, Usage, Classification, and Regression. Below the menu is a 'dabeaz' advertisement for advanced programming courses. The main content area has a blue header with 'Docs » Welcome to Lazy Predict's documentation!' and an 'Edit on GitHub' link. The main heading is 'Welcome to Lazy Predict's documentation!'. Under 'Contents:', there are links for Installation (with sub-links for Stable release and From sources), Usage, Classification, and Regression. Under 'Indices and tables', there are links for Index, Module Index, and Search Page. A 'Next' button is located at the bottom right. The footer contains copyright information for 2022, the revision number, and mentions that it was built with Sphinx using a theme from Read the Docs.

Lazy Predict

Example:

Use LazyClassifier on the **Breast Cancer Data Set**
(this is the example from the website)

Ranked by
Accuracy

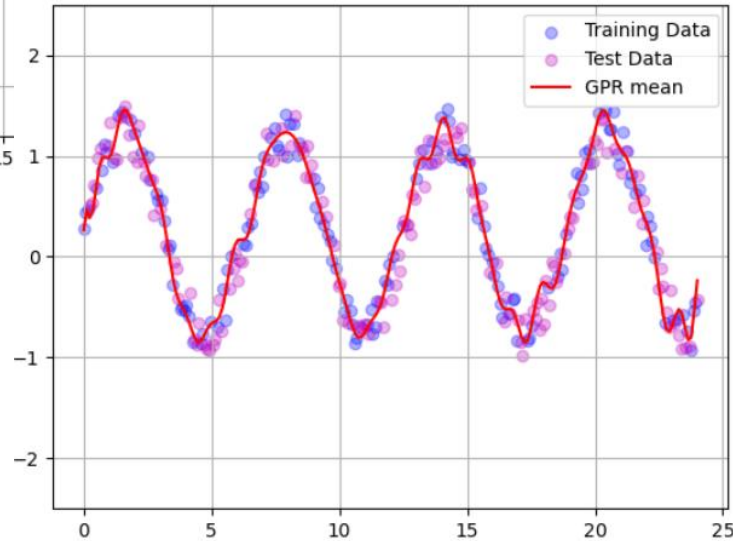
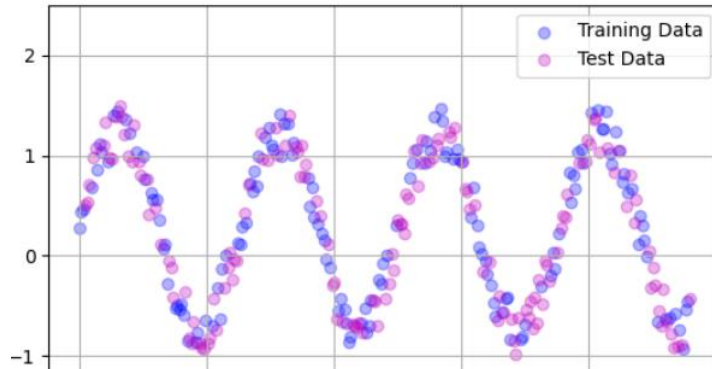


100% ██████████ 29/29 [00:01<00:00, 16.79it/s]						
Model	Accuracy	Balanced Accuracy	ROC AUC	F1 Score	Time Taken	
LinearSVC	0.99	0.99	0.99	0.99	0.02	
Perceptron	0.99	0.98	0.98	0.99	0.02	
LogisticRegression	0.99	0.98	0.98	0.99	0.03	
SVC	0.98	0.98	0.98	0.98	0.02	
XGBClassifier	0.98	0.98	0.98	0.98	0.13	
LabelPropagation	0.98	0.97	0.97	0.98	0.03	
LabelSpreading	0.98	0.97	0.97	0.98	0.03	
BaggingClassifier	0.97	0.97	0.97	0.97	0.07	
PassiveAggressiveClassifier	0.98	0.97	0.97	0.98	0.02	
SGDClassifier	0.98	0.97	0.97	0.98	0.02	
RandomForestClassifier	0.97	0.97	0.97	0.97	0.29	
CalibratedClassifierCV	0.98	0.97	0.97	0.98	0.07	
LGBMClassifier	0.97	0.97	0.97	0.97	0.17	
QuadraticDiscriminantAnalysis	0.96	0.97	0.97	0.97	0.03	
ExtraTreesClassifier	0.97	0.96	0.96	0.97	0.21	
RidgeClassifierCV	0.97	0.96	0.96	0.97	0.02	
RidgeClassifier	0.97	0.96	0.96	0.97	0.02	
AdaBoostClassifier	0.96	0.96	0.96	0.96	0.29	
KNeighborsClassifier	0.96	0.96	0.96	0.96	0.04	
BernoulliNB	0.95	0.95	0.95	0.95	0.02	
LinearDiscriminantAnalysis	0.96	0.95	0.95	0.96	0.03	
GaussianNB	0.95	0.95	0.95	0.95	0.02	
NuSVC	0.95	0.94	0.94	0.95	0.03	
ExtraTreeClassifier	0.94	0.93	0.93	0.94	0.02	
NearestCentroid	0.95	0.93	0.93	0.95	0.02	
DecisionTreeClassifier	0.93	0.93	0.93	0.93	0.02	
DummyClassifier	0.64	0.50	0.50	0.50	0.02	

Lazy Predict

Example:

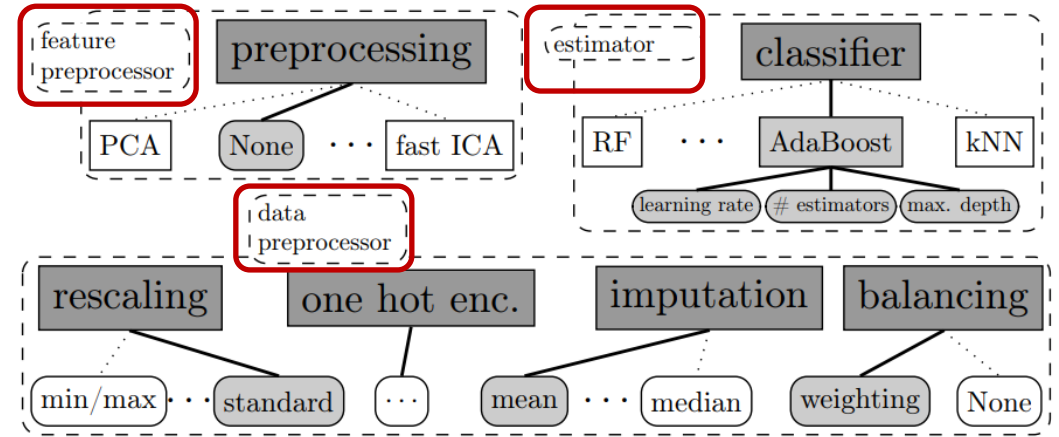
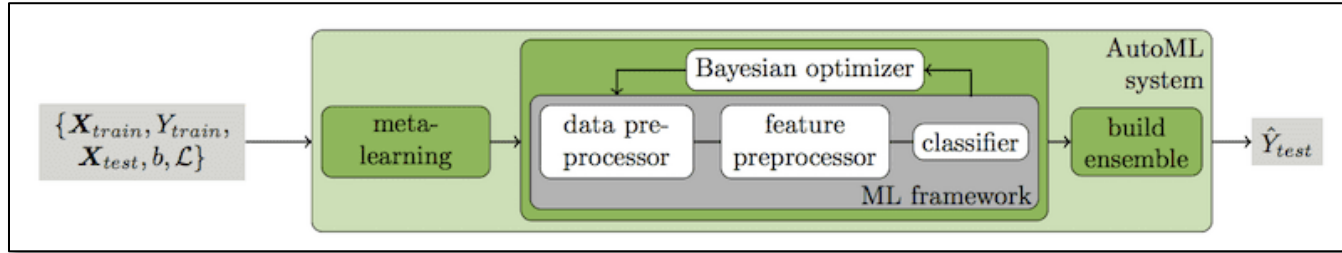
Use LazyRegressor on the **Sine Data Set**.



100% | 37/37 [00:01<00:00, 28.27it/s]

Model	Adjusted R-Squared	R-Squared	RMSE	Time Taken
GaussianProcessRegressor	0.95	0.95	0.16	0.03
KNeighborsRegressor	0.94	0.94	0.17	0.02
ExtraTreesRegressor	0.94	0.94	0.19	0.18
BaggingRegressor	0.93	0.93	0.19	0.05
GradientBoostingRegressor	0.93	0.93	0.20	0.08
ExtraTreeRegressor	0.91	0.91	0.22	0.01
DecisionTreeRegressor	0.91	0.91	0.22	0.01
XGBRegressor	0.90	0.90	0.23	0.07
HistGradientBoostingRegressor	0.78	0.78	0.34	0.10
LGBMRegressor	0.76	0.76	0.36	0.07
AdaBoostRegressor	0.55	0.56	0.49	0.08
NuSVR	0.12	0.12	0.69	0.02
SVR	0.11	0.11	0.70	0.02
MLPRegressor	0.04	0.05	0.72	0.10
LinearSVR	0.02	0.03	0.73	0.02
HuberRegressor	0.01	0.02	0.73	0.02
SGDRegressor	0.01	0.02	0.73	0.01
Lars	0.01	0.01	0.73	0.01
TransformedTargetRegressor	0.01	0.01	0.73	0.02
OrthogonalMatchingPursuit	0.01	0.01	0.73	0.01
LinearRegression	0.01	0.01	0.73	0.02
RidgeCV	0.01	0.01	0.73	0.02
TweedieRegressor	-0.00	0.00	0.74	0.01
BayesianRidge	-0.02	-0.01	0.74	0.02
ElasticNetCV	-0.02	-0.01	0.74	0.09
LassoLarsIC	-0.02	-0.01	0.74	0.01
LassoLarsCV	-0.02	-0.01	0.74	0.02
LassoLars	-0.02	-0.01	0.74	0.01
LassoCV	-0.02	-0.01	0.74	0.08
DummyRegressor	-0.02	-0.01	0.74	0.01
LarsCV	-0.02	-0.01	0.74	0.02
ElasticNet	-0.02	-0.01	0.74	0.01
Lasso	-0.02	-0.01	0.74	0.01
KernelRidge	-0.08	-0.07	0.76	0.01
PassiveAggressiveRegressor	-0.90	-0.89	1.02	0.02

Auto-Sklearn



- Feurer et al. (2015) and Feurer et al. (2022)
- <https://automl.github.io/auto-sklearn/master/>
- For regression and classification with pre-processing.
- A total of 110 tunable hyper-parameters across all models (2015).
- Can discover ensembles.
- Uses Bayesian Optimization and meta-learning.

Efficient and Robust Automated Machine Learning


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Abstract

The success of machine learning in a broad range of applications has led to an ever-growing demand for machine learning systems that can be used off the shelf by non-experts. To be effective in practice, such systems need to automatically choose a good algorithm and feature preprocessing steps for a new dataset at hand, and also set their respective hyperparameters. Recent work has started to tackle this *automated machine learning (AutoML)* problem with the help of efficient Bayesian optimization methods. Building on this, we introduce a robust new AutoML system based on scikit-learn (using 15 classifiers, 14 feature preprocessing methods, and 4 data preprocessing methods, giving rise to a structured hypothesis space with 110 hyperparameters). This system, which we dub AUTO-SKLEARN, improves on existing AutoML methods by automatically taking into account past performance on similar datasets, and by constructing ensembles from the models evaluated during the optimization. Our system won the first phase of the ongoing ChaLearn AutoML challenge, and our comprehensive analysis on over 100 diverse datasets shows that it substantially outperforms the previous state of the art in AutoML. We also demonstrate the performance gains due to each of our contributions and derive insights into the effectiveness of the individual components of AUTO-SKLEARN.

Optuna

- Akiba et al. (2019)
- Suitable for CASH (algorithm selection + hyper-parameter tuning)
- Models and hyper-parameters are user-defined.
- Uses Bayesian Optimization.



Optuna: A hyperparameter optimization framework

Akiba et al., (2019) Optuna: A Next-generation Hyperparameter Optimization Framework.
<https://arxiv.org/pdf/1907.10902.pdf>

Optuna has modern functionalities as follows:

- Lightweight, versatile, and platform agnostic architecture**
 - Handle a wide variety of tasks with a simple installation that has few requirements.
- Pythonic search spaces**
 - Define search spaces using familiar Python syntax including conditionals and loops.
- Efficient optimization algorithms**
 - Adopt state-of-the-art algorithms for sampling hyperparameters and efficiently pruning unpromising trials.
- Easy parallelization**
 - Scale studies to tens or hundreds of workers with little or no changes to the code.
- Quick visualization**
 - Inspect optimization histories from a variety of plotting functions.

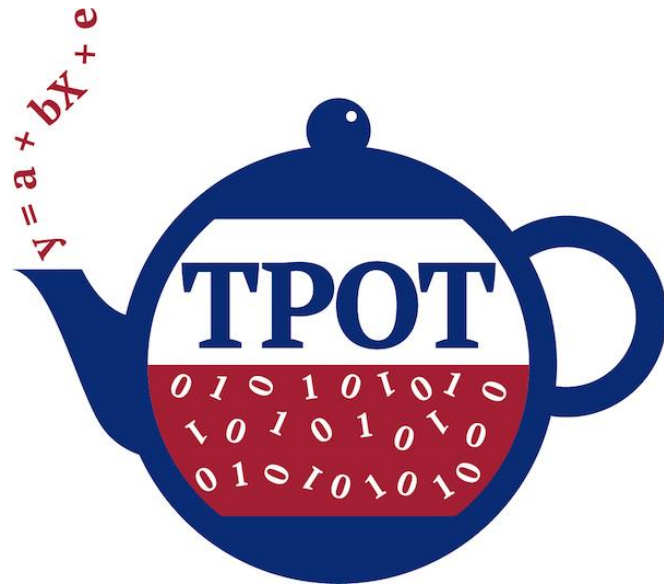
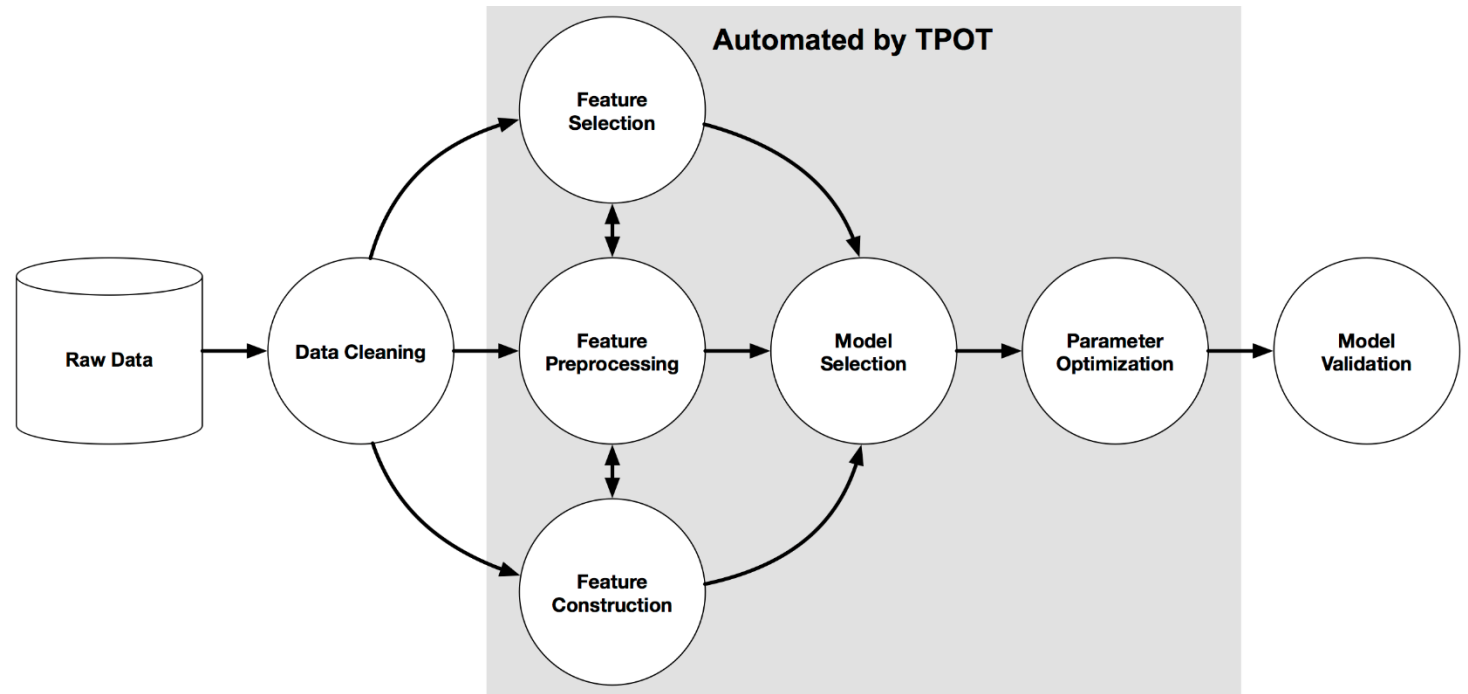
- Grid Search implemented in `GridSampler`
- Random Search implemented in `RandomSampler`
- Tree-structured Parzen Estimator algorithm implemented in `TPESampler`
- CMA-ES based algorithm implemented in `CmaEsSampler`
- Algorithm to enable partial fixed parameters implemented in `PartialFixedSampler`
- Nondominated Sorting Genetic Algorithm II implemented in `NSGAIISampler`
- A Quasi Monte Carlo sampling algorithm implemented in `QMCSampler`

The default sampler is `TPESampler`.

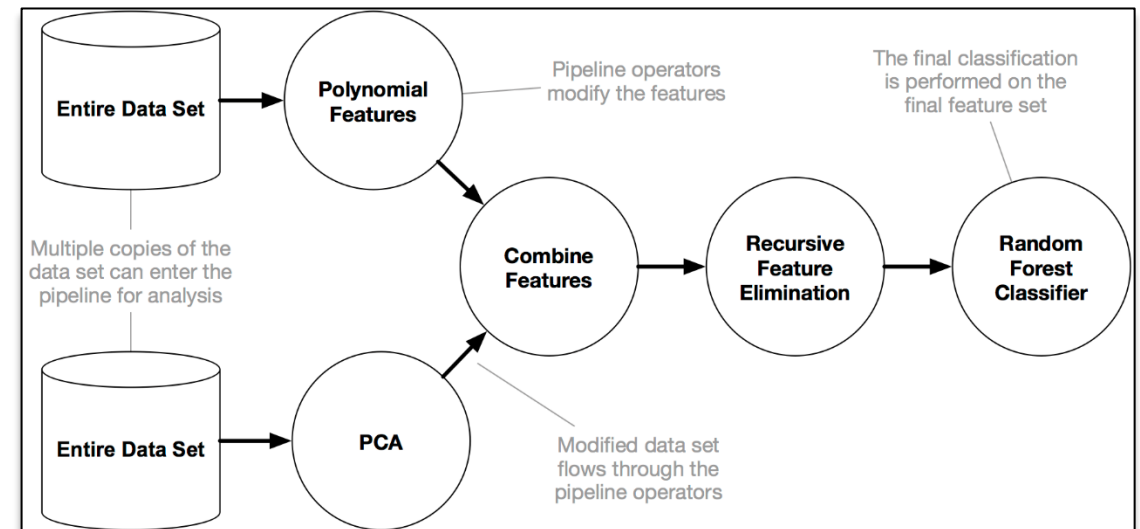
Main algorithm:
TPE (Tree-structured Parzen Estimator)
- A variant of Bayesian Optimization

TPOT

- Olson and Moore (2016)
- <http://epistasislab.github.io/tpot/>
- TPOT = **T**ree-based **P**ipeline **O**ptimization **T**ool
- TPOT optimizes machine learning pipelines using **genetic programming**.



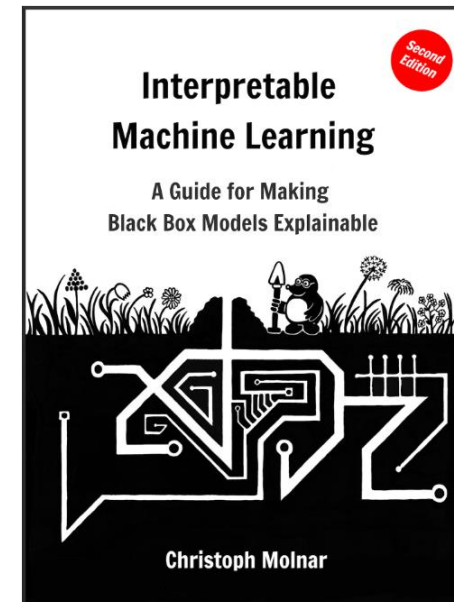
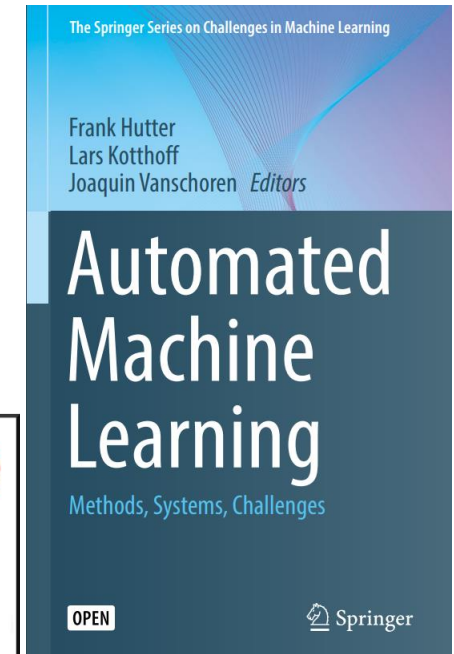
Sample Result:



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 - Shapley Additive Explanations

Hutter, Kotthoff,
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Molnar (2022)

Explainable AI (XAI)

IBM

What is explainable AI (XAI)?

Explainable artificial intelligence (XAI) is a set of processes and methods that allows human users to **comprehend and trust** the results and output created by machine learning algorithms. Explainable AI is used to describe an AI model, its expected **impact** and **potential biases**. It helps characterize model **accuracy, fairness, transparency** and outcomes in AI-powered decision making.

Explainable AI is crucial for an organization in building trust and confidence when putting AI models into production. AI explainability also helps an organization adopt a **responsible** approach to AI development.

- IBM (<https://www.ibm.com/watson/explainable-ai>)

Explainable AI (XAI)

Understandability

Ability of a model to make a human understand its *internal structure* and how it works *algorithmically*.

Comprehensibility

Ability of a learning algorithm to represent its learned knowledge in a human understandable fashion.

Interpretability

Refers to how accurate a machine learning model can associate a cause to an effect.

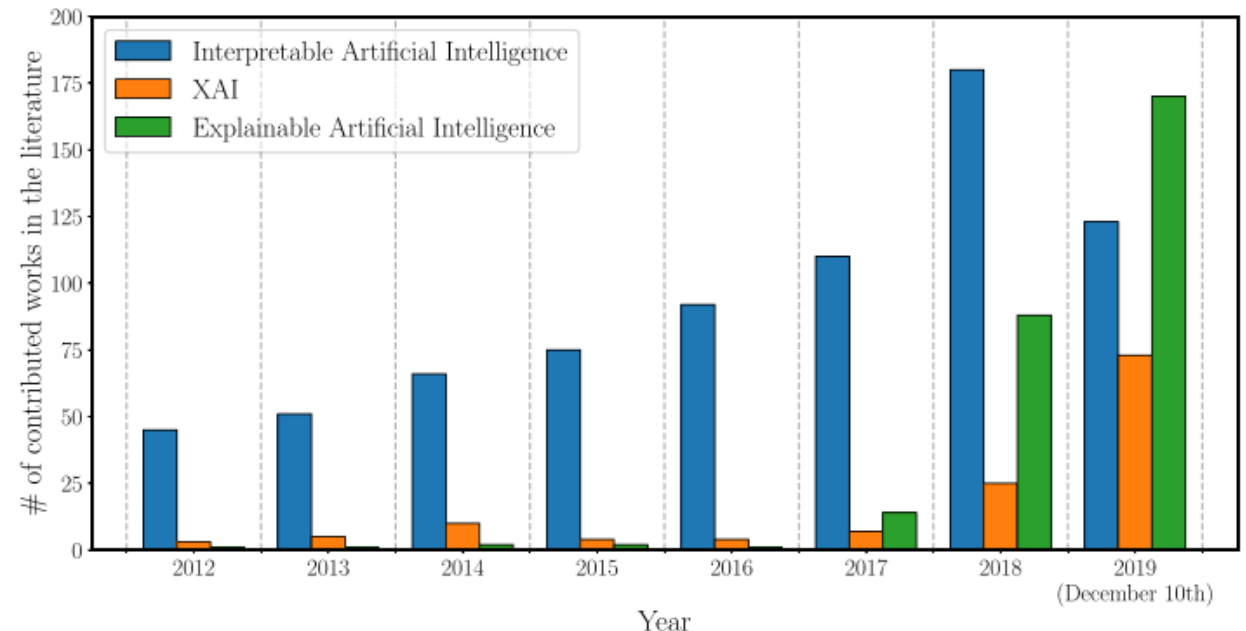
Transparency

A model is transparent if, by itself, it is already understandable.

Explainability

Ability of a model to explain its results to humans:

- How did it arrive at its decisions?
- Which inputs in the data prompted the decision to change?
- Which features have a significant effect on the prediction?



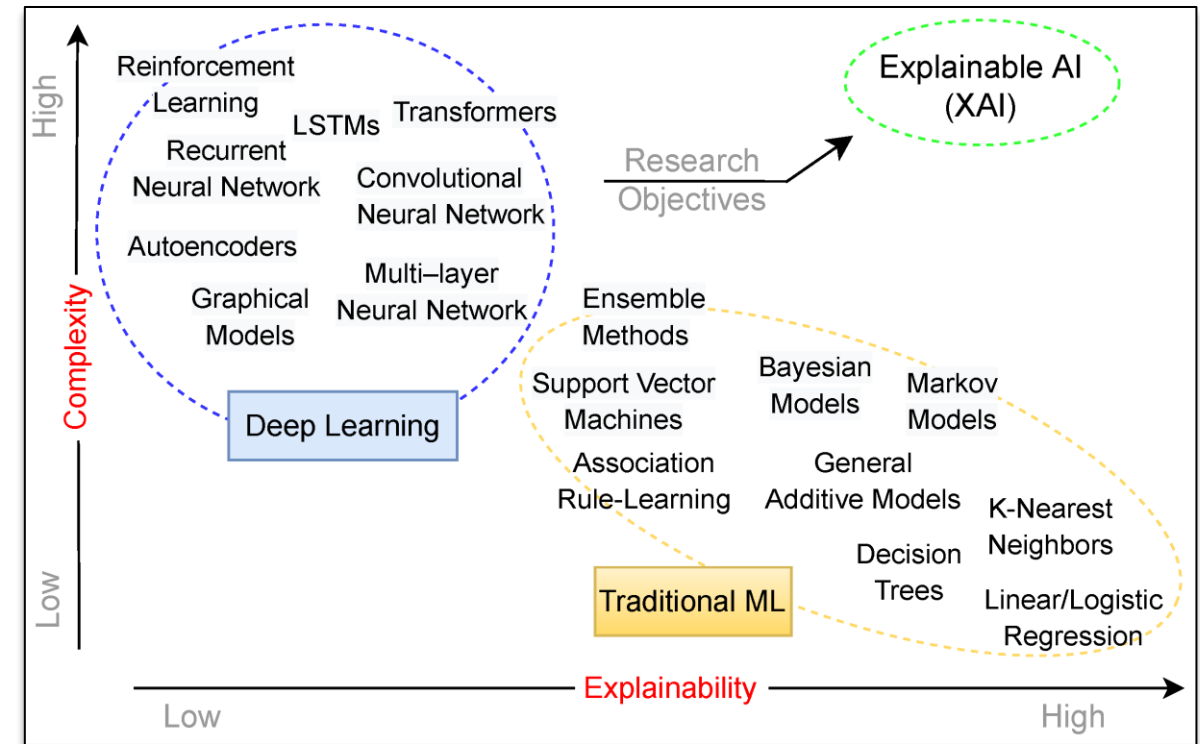
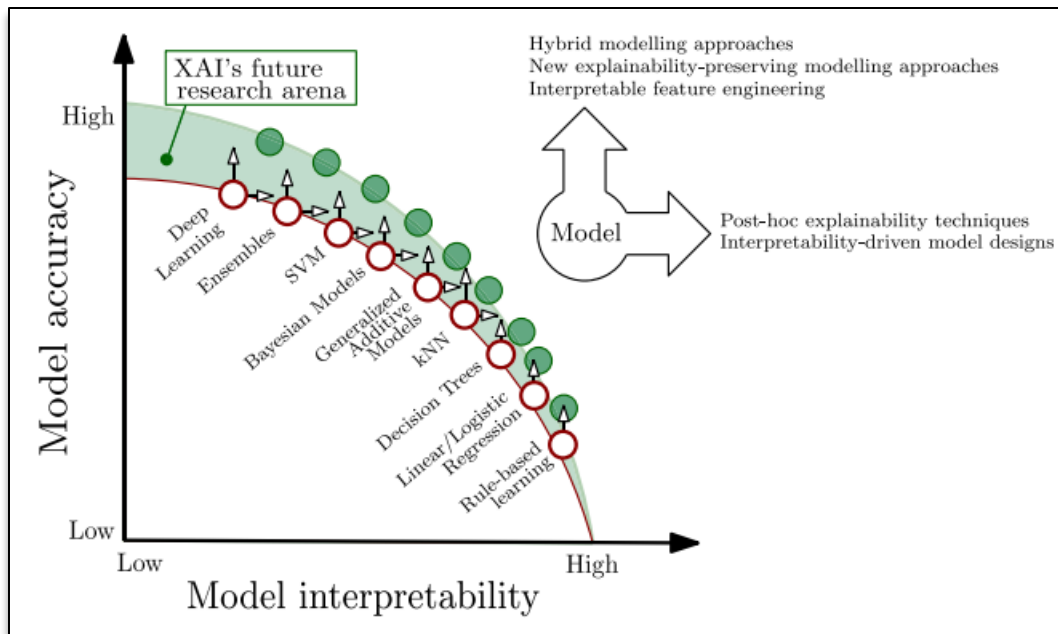
Number of Papers in Literature that mentioned XAI

Reference: Arrieta et al. (2020). Explainable Artificial Intelligence (XAI): Concepts, taxonomies, opportunities and challenges toward responsible AI. Information Fusion, Vol. 58, June 2020, 82-115.

<https://doi.org/10.1016/j.inffus.2019.12.012>

Explainable AI (XAI)

- It is said that traditional ML models are explainable, but are low-performing.
- On the other hand, deep learning models are not explainable but high-performing.
- Explainable AI aims to provide models that are *explainable yet high-performing*.



Reference: Clement, T.; Kemmerzell, N.; Abdelaal, M.; Amberg, M. XAIR: A Systematic Metareview of Explainable AI (XAI) Aligned to the Software Development Process. Mach. Learn. Knowl. Extr. 2023, 5, 78-108. <https://doi.org/10.3390/make5010006>

Reference: Arrieta et al. (2020). Explainable Artificial Intelligence (XAI): Concepts, taxonomies, opportunities and challenges toward responsible AI. Information Fusion, Vol. 58, June 2020, 82-115. <https://doi.org/10.1016/j.inffus.2019.12.012>

How to Explain ML models?

Intrinsically Explainable

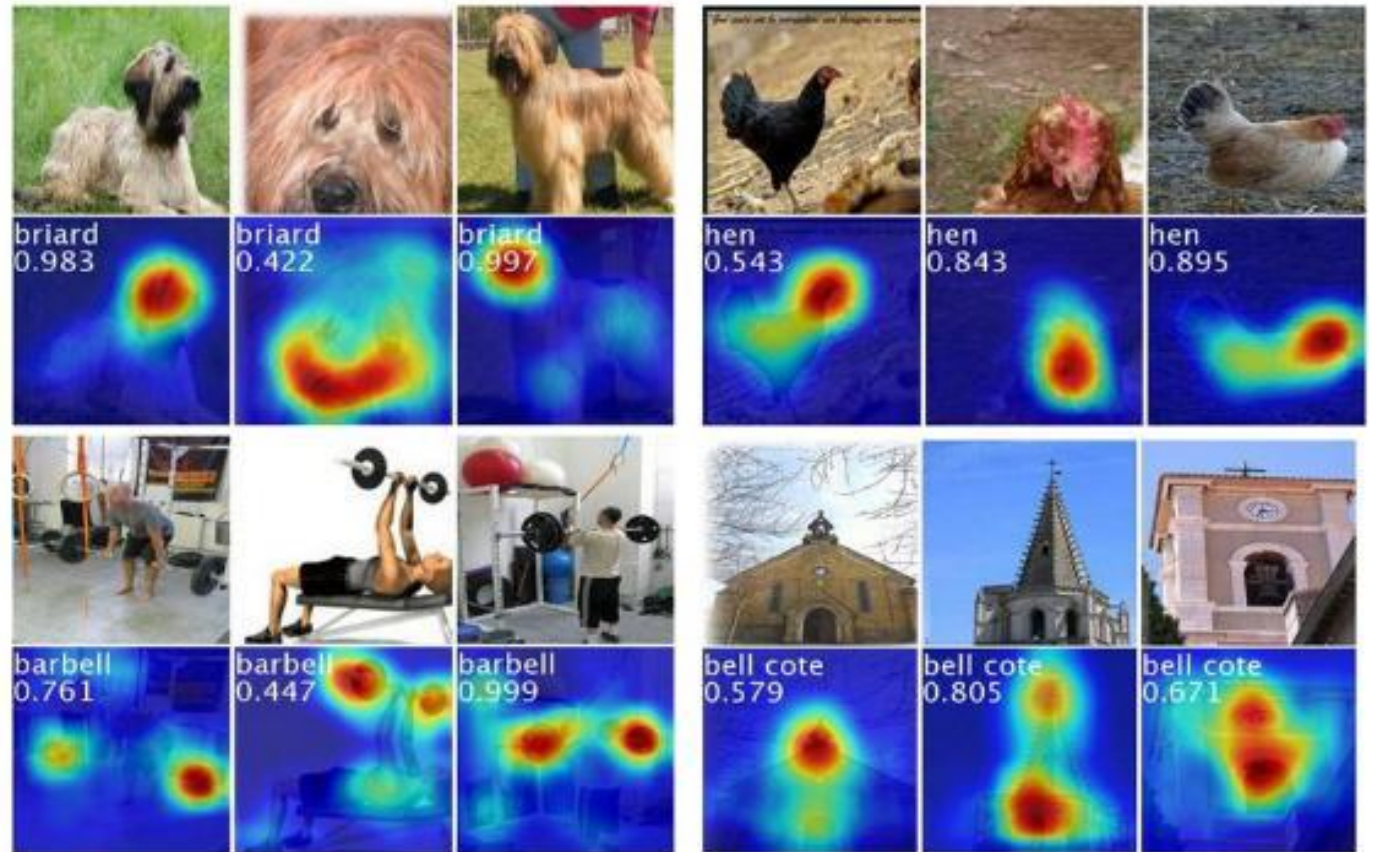
Some models are explainable / interpretable on their own.

Post-hoc Explainability

If an ML model is not transparent, additional analysis must be done *after training the model* in order to provide an explanation.

Some examples of **post-hoc explainability** methods:

- Visual explanation
- Saliency maps (images)
- Model simplification
- Uncertainty Quantification
- **Look at the Features!**
 - Feature Importance
 - Feature Relevance
 - Feature Attribution
 - Feature Significance



<https://debuggercafe.com/saliency-maps-in-convolutional-neural-networks/>

How to Explain ML models?

ML explainers can be categorized into:

Model-specific Explainers

The explainability method is only applicable to a certain ML model only.

vs.

Model-agnostic Explainers

The explainability method is applicable to any ML model.

Local Explainers

An explanation is provided for a specific data sample only.

vs.

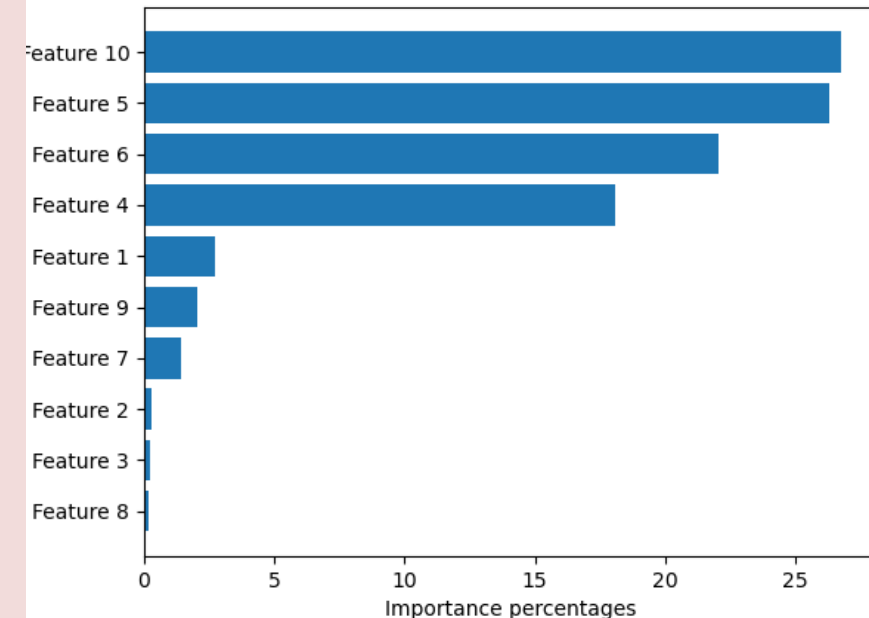
Global Explainers

An explanation is provided for the model behavior across the entire data space.

Feature Importance

- A mechanism to identify features that have the most *relevant impact* to the model predictions.
- Typically model-agnostic; can be local or global
- Packages: LIME, SHAP, DeepLIFT, etc.

Sample Result



How to Explain ML models?

Permutation Feature Importance (PFI)

- PFI is defined as the decrease in the model score when a single feature value is **randomly shuffled**.
- If 2 or more features are correlated, PFI is biased to give them lower importance. Cluster correlated features first, then pick only one from each cluster to shuffle.

- Inputs: fitted predictive model m , tabular dataset (training or validation) D .
- Compute the reference score s of the model m on data D (for instance the accuracy for a classifier or the R^2 for a regressor).
- For each feature j (column of D):
 - For each repetition k in $1, \dots, K$:
 - Randomly shuffle column j of dataset D to generate a corrupted version of the data named $\tilde{D}_{k,j}$.
 - Compute the score $s_{k,j}$ of model m on corrupted data $\tilde{D}_{k,j}$.
 - Compute importance i_j for feature f_j defined as:

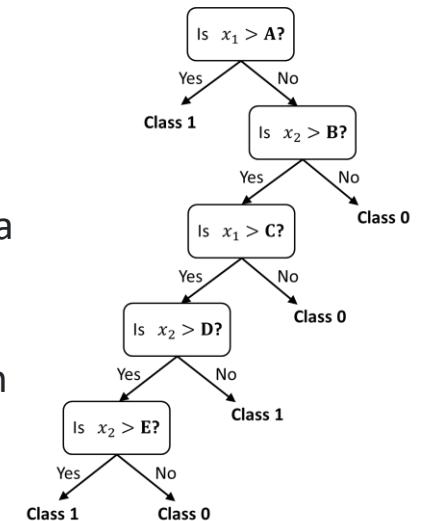
$$i_j = s - \frac{1}{K} \sum_{k=1}^K s_{k,j}$$

Drop-Column Feature Importance

- Defined as the decrease in the model score when a **single feature is removed** from the data set.
- Requires model to be re-trained. Hence, it is not purely a post-hoc explainer.

Mean-Decrease-in-Impurity Feature Importance

- Applicable to **tree-based models** only (e.g. Random Forest)
- Idea: Features used at the top of the tree contribute to the final prediction decision of a larger fraction of the input samples.
- “Decrease in impurity” quantifies the fraction of the samples a feature contributes to.



How to Explain ML models?

Shapley Additive Explanations (SHAP)

- Uses “Shapley values” from coalitional game theory.
- Feature importance, I_j , is computed as:

$$I_j = \sum_{i=1}^n |\phi_j^{(i)}|$$

where ϕ is the Shapley value (contribution of the j th feature at the i th sample).

- Calculation of the Shapley value involves iterating over **all possible subsets** of the feature set, then checking the changes in the model score.
- Computation time grows exponentially with the number of features. Hence, we can approximate the Shapley value using only local samples → **Kernel SHAP**.

Shapley values are calculated as:

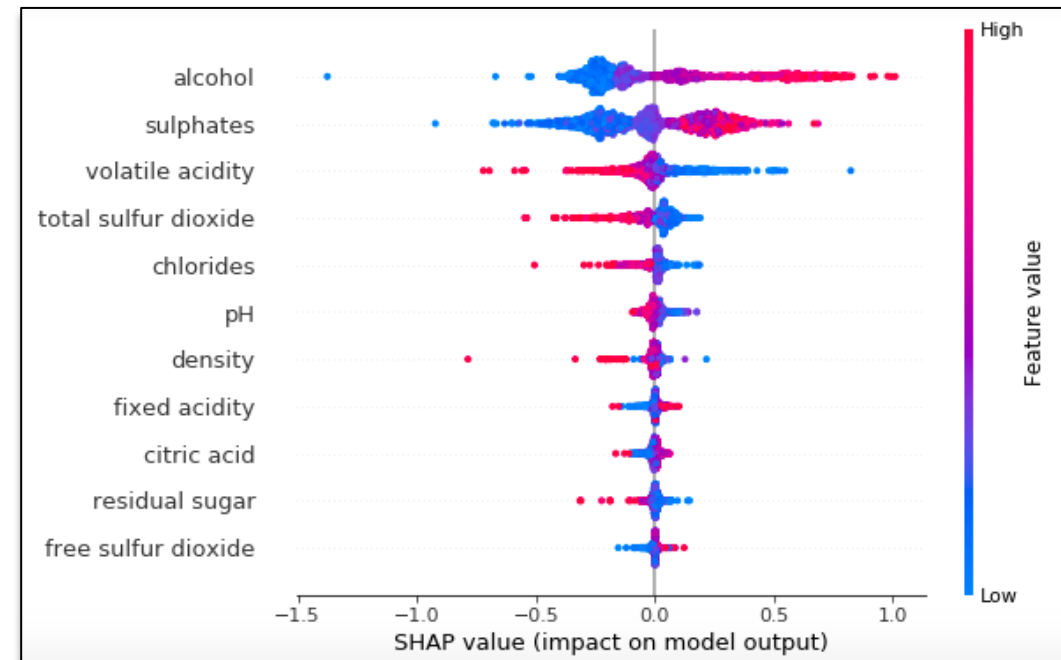
$$\phi_j = \sum_{S \in j} \frac{|S|! (|F| - |S| - 1)!}{|F|!} [f_{S \cup j}(x_{S \cup j}) - f_S(x_S)]$$

F = set of all input features

S = coalition which is a subset of F

$|\cdot|$ = cardinality of the set

$f_{S \cup j}(x_{S \cup j}) - f_S(x_S)$ = marginal contribution of feature j in coalition S .

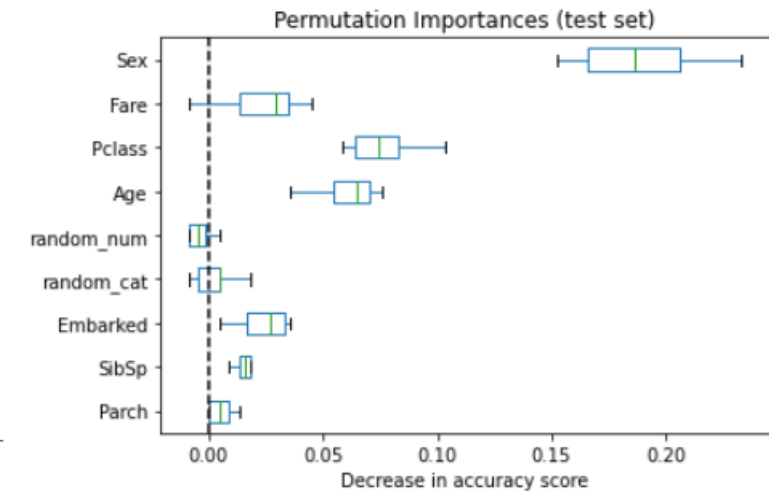
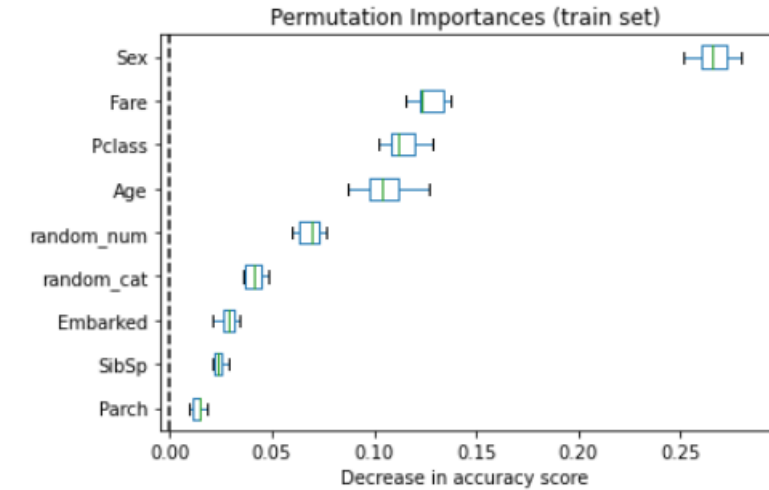
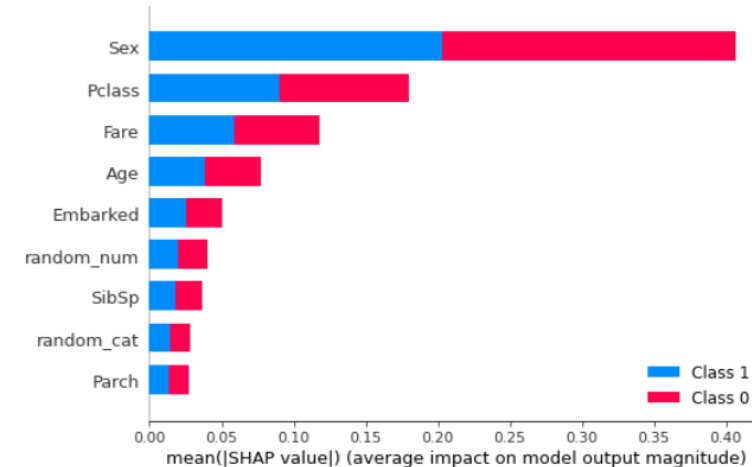
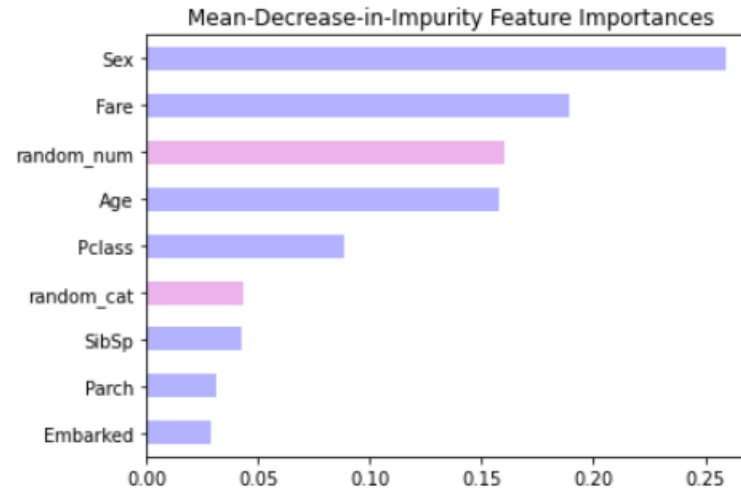


How to Explain ML models?

Example:

Apply feature importance techniques on a Random Forest classifier trained on the Titanic data set.

Type of feature	Feature	Feature values
	Survived	If survived or no (0 = No, 1 = Yes) (Target variable)
Numeric variables	PassengerId	Unique ID of each passenger (in integers)
	Age	Age in years
	SibSp	Number of siblings / spouses aboard the Titanic
	Parch	Number of parents / children aboard the Titanic
	Fare	Passenger fare
Strings:	Name	Name of passenger
	Cabin	Cabin number
	Ticket	Ticket number
Categorical variables:	Pclass	Ticket class (1 = 1st, 2 = 2nd, 3 = 3rd)
	Sex	Sex (string : 'male' 'female')
	Embarked	Port of Embarkation (C = Cherbourg, Q = Queenstown, S = Southampton)

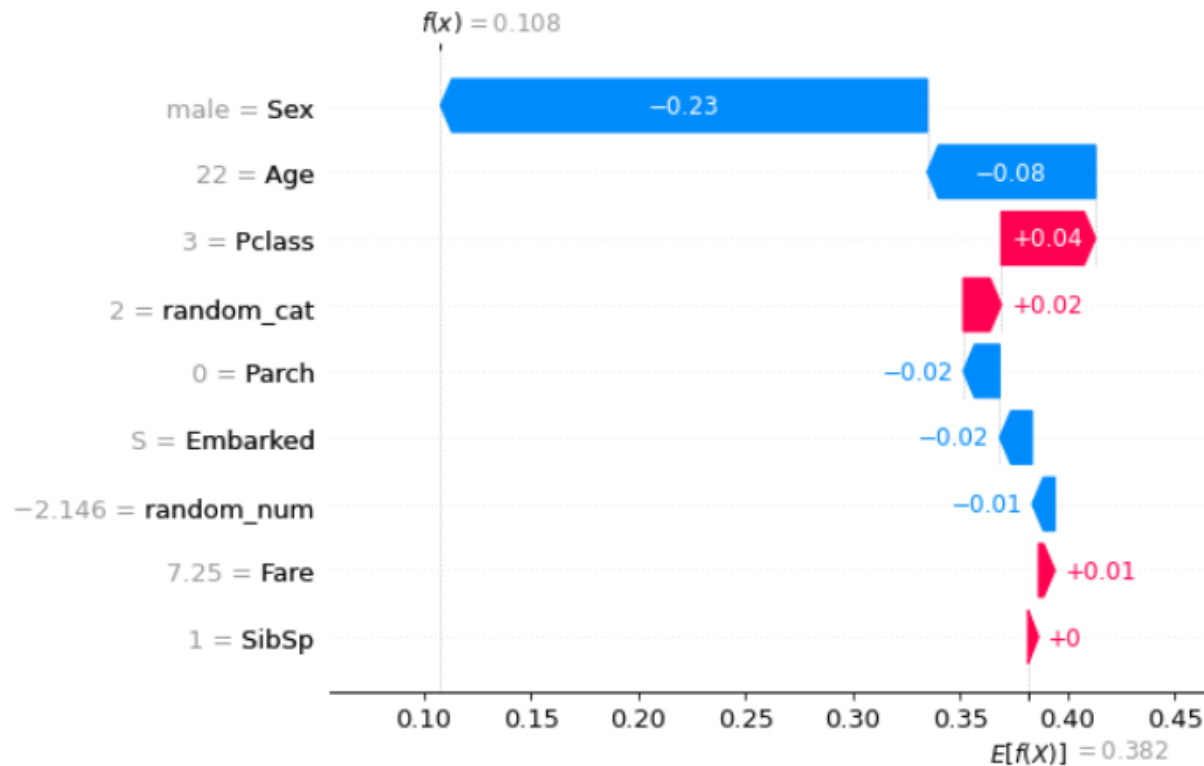


How to Explain ML models?

Example: Titanic Data Set – Local Explanations

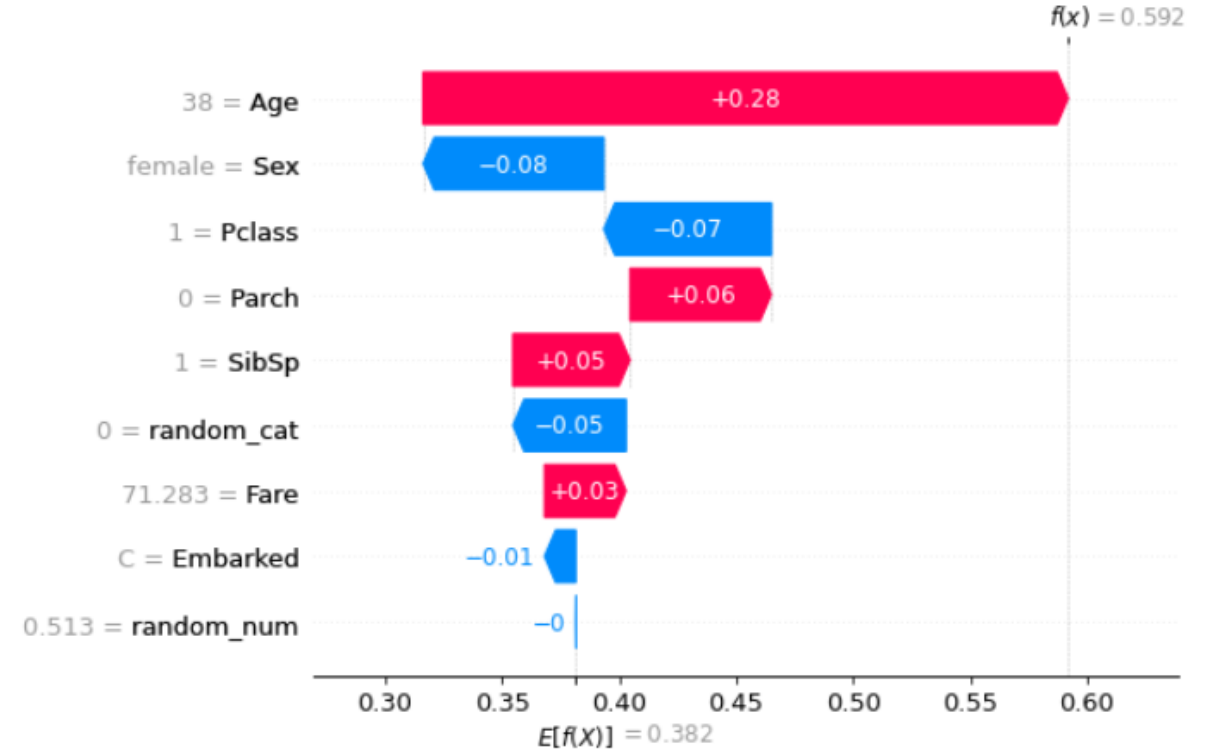
Passenger 288

Random Forest Prediction: Did not survive



Passenger 869

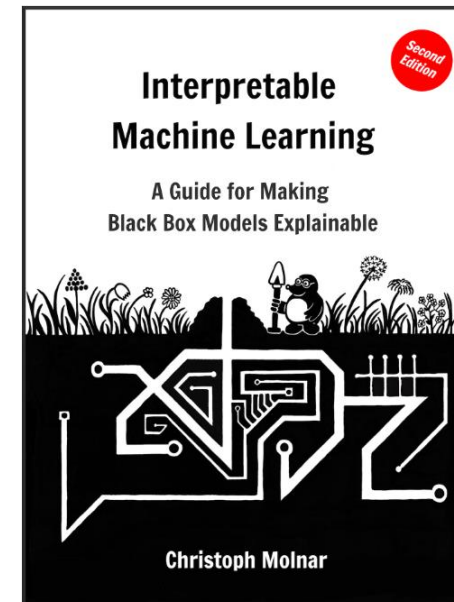
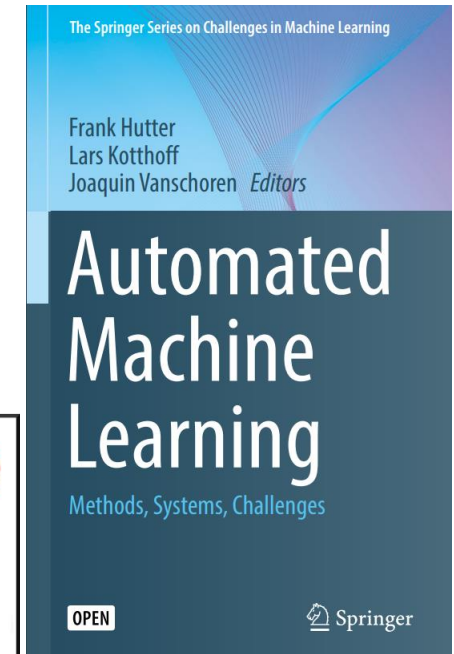
Random Forest Prediction: Survived



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Hutter, Kotthoff,
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Molnar (2022)

Further Reading

- <https://www.automl.org/automl/>
- https://www.automl.org/wp-content/uploads/2019/05/AutoML_Book.pdf
- <https://docs.h2o.ai/h2o/latest-stable/h2o-docs/automl.html>
- <https://machinelearningmastery.com/auto-sklearn-for-automated-machine-learning-in-python>
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