

Machine learning (ML) is a field of Artificial Intelligence (AI) and a field of inquiry devoted to understanding and building methods that 'learn', that is, methods that leverage data to improve performance on some set of tasks. [1]

Common application scenarios:

- (1) Self Driving Cars
- (2) Recommending Systems
- (3) Automated Translation
- (4)

For Insurance:

- (1) Predict future claim frequency/severity
- (2) Fraud prevention
- (3) ..



Fig. Self-Driving Cars [2]

However, ML tasks can be **experience-dependent** and **heavy manual work**.

Given the nature of ML algorithms, which are **data-driven**, selection of models and hyperparameters are critical for each dataset, and **no universal solution** exists.

Furthermore, industrial datasets usually are not well-formatted or well-organized, and problems like **missing values**, **irrelevant features**, **imbalance distributions** exists.

It's difficult for those who have no previous experience/knowledge to gain hands-on experience.



Automated Machine Learning (AutoML) is one of the solutions.

AutoML tries to automatically select a ML model and tuning for optimal hyperparameters, so that "non-expert users" can apply ML to their application scenarios more effectively and "achieve improved performance". [3]

```
save_path = 'agModels-predictClass' # specifies folder to store trained models
predictor = TabularPredictor(label=label, path=save_path).fit(train_data)
```

Fig. AutoGluon [4]

```
import autosklearn.classification
cls = autosklearn.classification.AutoSklearnClassifier()
cls.fit(X_train, y_train)
predictions = cls.predict(X_test)
```

Fig. auto-sklearn [5]

```
>>> import autoPyTorch
>>> cls = autoPyTorch.api.tabular_classification.TabularClassificationTask()
>>> cls.search(X_train, y_train)
>>> predictions = cls.predict(X_test)
```

Fig. Auto-PyTorch [6]



^[3] Thornton, C., Hutter, F., Hoos, H. H., & Leyton-Brown, K. (2013, August). Auto-WEKA: Combined selection and hyperparameter optimization of classification algorithms. In Proceedings of the 19th ACM SIGKDD international conference on Knowledge discovery and data mining (pp. 847-855).

^{.]} https://auto.gluon.ai/stable/index.html

^[5] https://automl.github.io/auto-sklearn/master/

^[6] https://automl.github.io/Auto-PyTorch/development/

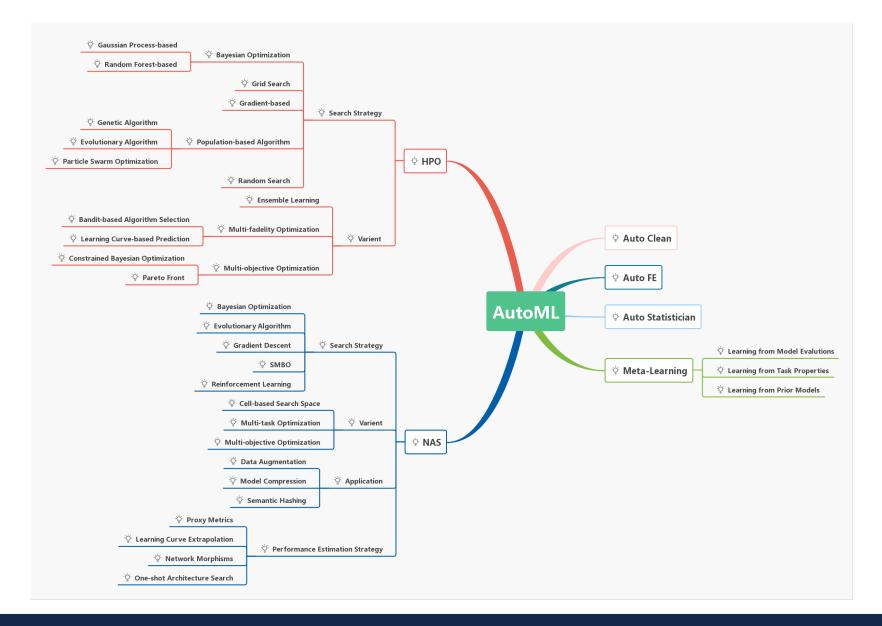


Fig. AutoML research mainstream [7]

Key criteria of AutoML:

(1) Better Performance

What's a proper search space; How the model/hyperparameter evaluated; Better model search algorithms, hyperparameter optimization algorithms; ...

(2) Higher Efficiency

AutoML usually evaluate by training multiple models, how to more efficiently assess (or sometimes with limited computation resources)

(3) Ease of use, Robustness

The goal is to ease expertise required, a robust AutoML for all possible scenarios



Our AutoML pipeline:

- (1) Complete, fully functional processing and model tuning
- (2) Special treatment for imbalanced datasets
- (3) Record training process and store the optimal pipeline for continued applications



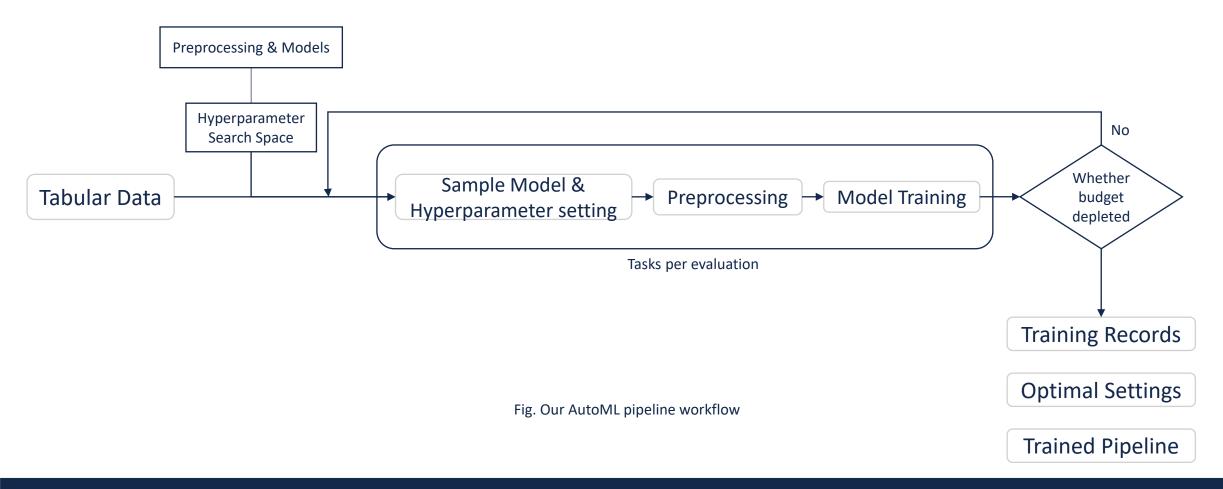
2. Components & Pipline

- 1. Data Encoding
- 2. Data Imputation
- 3. Data Balancing
- 4. Data Scaling
- 5. Feature Selection
- 6. Classification/Regression Models
- 7. Model Selection and Hyperparameter Optimization

Preprocessing

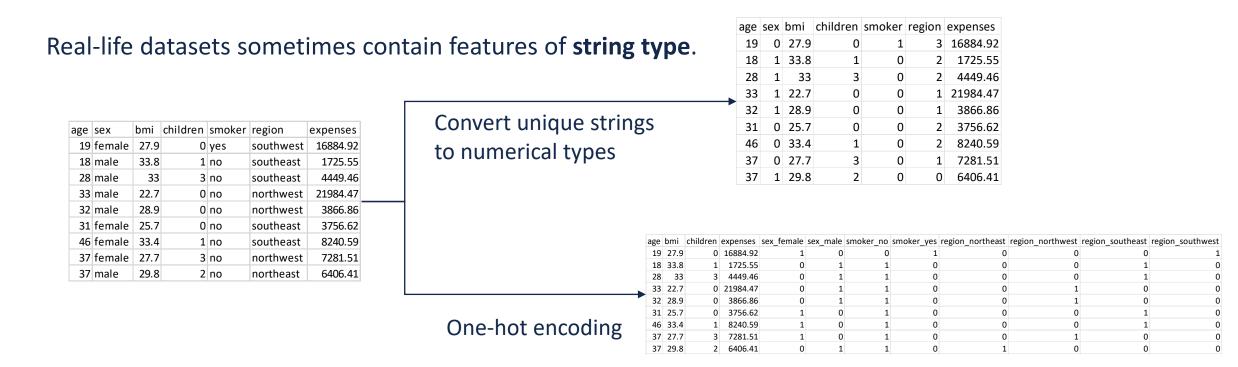


2. Components & Pipeline





2.1. Data Encoding



Majority of common ML methods in Python does not support string as inputs, encoding becomes necessary.



Some of datasets contains missing values where true values can not be traced.

Causes: Incomplete data entry, Save malfunction, ...

Common solutions:

(1) Delete missing values.

Advantage: all remaining values are true values.

Drawback: not feasible when data size is small.

(2) Impute the missing values with estimated values.

Advantage: best utilize all available information.

Drawback: imputed values may not accurately describe the missing values, time-consuming, ...



Incorporated imputation methods:

2.2.1. Simple Imputation

Most common and efficient imputation methods. Use non-missing summary statistics (mean/median/...) to fill the missing values.

Drawback: Indifferent to the variation of other information.

2.2.2. Joint Imputation

Assume all features follow some multi-variate distributions, whose parameters (e.g., mean vector μ and covariance matrix Σ in multi-normal distributions) are determined by observed values.

Drawback: Ideal assumption of joint distribution usually do not exist.



Incorporated imputation methods:

2.2.3. Expectation Maximization (EM) [8]

Utilize the classical EM algorithm, where the E step tries to create a function of log-likelihood, and M step tries to maximize the likelihood.

Drawback: underestimate standard error of imputed values.

2.2.4. KNN Imputation [9]

2.2.5. Miss Forest Imputation [9]

2.2.4, 2.2.5 builds corresponding models (k Nearest Neighbors for 2.2.4 and Random Forest for 2.2.5) on observed values and predictions as imputation values.



Incorporated imputation methods:

2.2.6. Multiple Imputation by Chained Equations (MICE) [10]

One of most popular Multiple Imputation methods, multiple copies datasets are created and each missing values are filled with multiple cycles of predictions of model fitted.

Drawback: Time-consuming for not small datasets to converge.

2.2.7. Generative Adversarial Imputation Nets (GAIN) [11]

Utilize the Generative Adversarial Network (GAN) to train a Generator (G) and Discriminator (D) where G tries to generate values for missing positions and D tries to distinguish whether the generated values are valid.

Drawback: Large data size required for neural network training, and time-consuming.



Some of datasets exhibits **imbalanced nature** where majority values are the same (e.g., 99% of policyholders do not report claims).

Traditional ML models evaluated by classical metrics may not be the ideal solution by the business perspective.

Common solutions:

- (1) Increase the weights of minority class.
- (2) Over-sampling on minority class/Down-sampling on majority class. [12]
- (3) Create a model ensemble (multiple models weighted on prediction).
- (4) Special loss metrics for gradient-based models.
- (5) ...

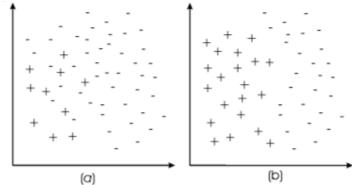


Fig. Spatial illustration of unbalanced datasets (a) and balanced datasets (b). [12]

Incorporated balancing methods: (focusing on over-sampling/down-sampling at this step)

2.3.1. Simple Random Over-Sampling

2.3.2. Simple Random Down-Sampling

Method 2.3.1 and 2.3.2 simply randomly copy minority class entries/eliminate majority class entries.

2.3.3. Tomek Link [13]

An Under-Sampling method. Remove noise majority class around decision boundaries.

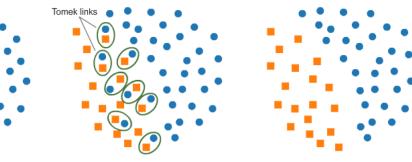


Fig. Illustration of Tomek Link [14]

Incorporated balancing methods: (focusing on over-sampling/down-sampling at this step)

2.3.4. Edited Nearest Neighbors (ENN) [15]

An Under-Sampling method.

Remove majority class observations which disagree with predictions from kNN model.

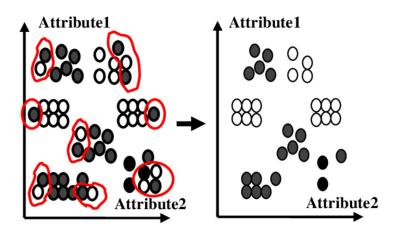


Fig. Illustration Edited Nearest Neighbor [16]

2.3.5. Condensed Nearest Neighbors (CNN) [17]

An Under-Sampling method.

Select a subset of observations $\widehat{E} \subseteq E$ where \widehat{E} can predict all observations correctly using 1-NN.

[17]

Incorporated balancing methods:

(focusing on over-sampling/down-sampling at this step)

2.3.6. Synthetic Minority Over-Sampling Technique (Smote) [18]

A common Over-Sampling method.

Try to generate more realistic synthetic minority observations by interpolation between minority observations.

- 2.3.7. One Sided Selection (OSS): Tomek Link + CNN
- 2.3.8. CNN_Tomek Link: CNN + Tomek Link
- 2.3.9. Smote_Tomek Link: Smote + Tomek Link
- 2.3.10. Smote_ENN: Smote + ENN

Combination of two-step balancing methods, take advantages of both steps.

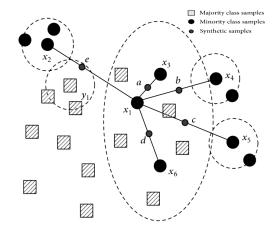


Fig. Illustration of Smote [19]



[18] [19]

2.4. Data Scaling

Scaling intends to transform data to fit specific scale so it may converge more easily.

Incorporated Scaling methods:

2.4.1. Standardize

All features are standardized using $(x - \bar{x})/\sigma_x$ where \bar{x} is the mean, σ_x is the standard deviation.

2.4.2. Normalize

Feature are normalized using x/x_{max} into unit scale.

2.4.3. Robust Scaling

Feature are scaled by range of two feature quantiles.

(e.g., scaled by the range between 25th quantile and 75th quantile)



2.4. Data Scaling

Incorporated Scaling methods:

2.4.4. Min-Max Scaling

Feature are scaled by min/max values to [0,1] range.

2.4.5. Power Transformer

Apply a power transformation (Box-Cox/Yeo-Johnson transformation) to each feature to shape data more normal-distributed.

2.4.6. Winsorization

Cap features at certain quantile to avoid extreme values (outliers).



Modern datasets have hundreds of (or even more) features with exploding size.

However, some of them may be reductant or irrelevant, which may decrease the model performance while still takes long training time. One of the solution is using **feature selection** to select only subset of features for model training.

Common categories of feature selection [20]:

- 1. Filter: use statistical analysis in only feature space
- 2. Wrapper: train a model on feature subsets and use performance as selection criteria.
- 3. Embedded: embed feature importance into model training and use as selection criteria.
- 4. **Hybrid:** combine filter and wrapper for feature selection.



[20]

Incorporated Feature Selection methods:

2.5.1. Feature Filter

Feature filter select relevant features by scoring features and selecting highest score features.

(1) Pearson Correlation Coefficient

$$R(i) = \frac{Cov(X_i, Y)}{\sqrt{Var(X_i)Var(Y)}}$$

(2) Mutual Information I(X,Y) = H(Y) - H(Y|X) using Shannon Entropy

$$H(Y) = -\sum_{y} p(y) \log(p(y)), H(Y|X) = -\sum_{x} \sum_{y} p(x, y) \log(p(y|x))$$



Incorporated Feature Selection methods:

2.5.2. Adaptive Sequential Forward Floating Search (ASFFS) [21]

ASFFS is a variation of sequential feature selection (SFS) method to deal with feature correlation.

ASFFS iteratively performs forward phase and backward until target reached where forward phase adds features, backward phase removes features.

ASFFS will adaptively change number of features consider at a time.

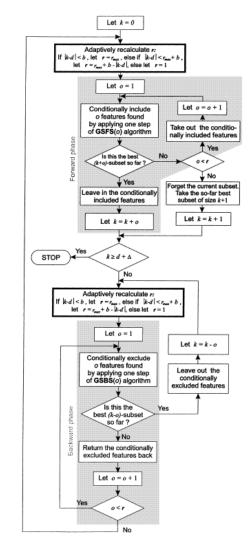


Fig. Workflow of ASFFS [21]

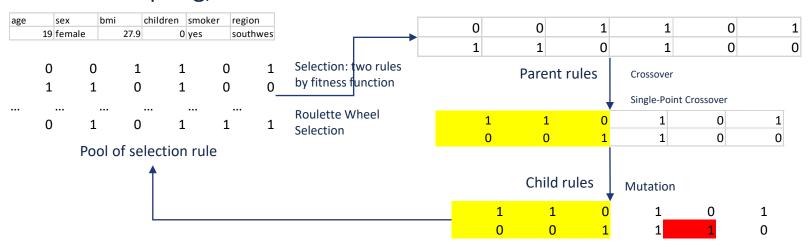


Incorporated Feature Selection methods:

2.5.3. Genetic Algorithm (GA) [22]

GA is a popular algorithm inspired by natural DNA replication/mutation.

GA consists of selection, crossover and mutation phase at each generation. With generations of offspring, best feature selection rules will be selected.



During the process, all rules are evaluated by fitness function with their performance and assigned a possibility of selection.

Incorporated Feature Selection methods:

2.5.4. minimal-Redundancy-Maximal-Relevance (mRMR) [23] [24] [25]

mRMR is a filter method, and a variation of SFS to both maximize relevance and minimize redundancy among selected features. Both redundancy and relevance are defined as mutual information.

2.5.5. Copula-based Feature Selection (CBFS) [26] [27]

CBFS is a filter method where the data is described using copulas, which is a popular method to describe multivariate correlation.

Features are scored by mutual information of copula values.



Peng, H., Long, F., & Ding, C. (2005). Feature selection based on mutual information criteria of max-dependency, max-relevance, and min-redundancy. IEEE Transactions on pattern analysis and machine intelligence, 27(8), 1226-1238.

^[25] Li, Z. (2022). A Feature Selection Method Using Dynamic Dependency and Redundancy Analysis. Arabian Journal for Science and Engineering, 1-15.

Lall, S., Sinha, D., Ghosh, A., Sengupta, D., & Bandyopadhyay, S. (2021). Stable feature selection using copula based mutual information. Pattern Recognition, 112, 107697.

^[26] Lall, S., & Bandyopadhyay, S. (2019, September). An I1-Norm regularized copula based feature selection. In Proceedings of the 2019 3rd International Symposium on Computer Science and Intelligent Control (pp. 1-6).

Incorporated Classification models:

Z.O.I.I. LUGISTIC REGIESSIO	2.6.1.1.	Logistic Regression
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- 2.6.1.2. Adaboost [28]
- **2.6.1.3.** Hist Gradient Boosting
- **2.6.1.4.** Linear Support Vector Machine (SVM) [30]
- 2.6.1.5. Kernel Support Vector Machine (SVM) [31]

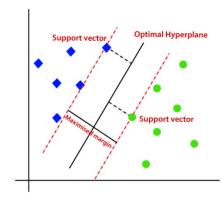


Fig. Support Vector Machine [32]



[28]

[31]

^[30] Fan, R.-E., Chang, K.-W., Hsieh, C.-J., Wang, X.-R. & Lin, C.-J. Liblinear: A library for large linear classification. the Journal of machine Learning research 9, 1871–1874 (2008).

Chang, C.-C. & Lin, C.-J. Libsvm: a library for support vector machines. ACM transactions on intelligent systems and technology (TIST) 2, 1–27 (2011).

^[32] https://medium.com/@viveksalunkhe80/support-vector-machine-svm-88f360ff5f38

Incorporated Classification models:

2.6.1.6. Decision Tree

2.6.1.7. Extra Trees

2.6.1.8. Random Forest

2.6.1.9. K Nearest Neighbors

2.6.1.10. SGD

[29]

[41]

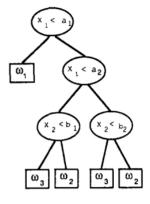
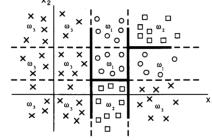


Fig. Decision Tree Split [29]





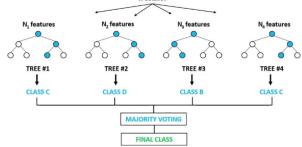


Fig. Random Forest [41]

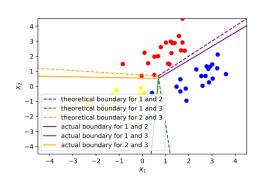
Incorporated Classification models:





- **2.6.1.13.** Bernoulli Naïve Bayes
- **2.6.1.14.** Gaussian Naïve Bayes
- 2.6.1.15. Multinomial Naïve Bayes

Fig. Linear Discriminant Analysis



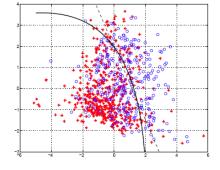


Fig. Quadratic Discriminant Analysis [42]



[42]

Incorporated Classification models:

2.6. 1	L.16.	Multi-Laye	r Perception	(MLP)	
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- 2.6.1.17. Passive Aggressive
- 2.6.1.18. Light Gradient Boosting Machine (LightGBM) [36]
- 2.6.1.19. Extreme Gradient Boosting (XGBoost) [37]
- 2.6.1.20. Generalized Additive Models (GAM) [38]

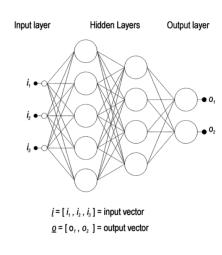


Fig. Multi-Layer Perceptron [33]



[33]

[37]

^[36] Ke, G., Meng, Q., Finley, T., Wang, T., Chen, W., Ma, W., ... & Liu, T. Y. (2017). Lightgbm: A highly efficient gradient boosting decision tree. Advances in neural information processing systems, 30.

Chen, T., & Guestrin, C. (2016, August). Xgboost: A scalable tree boosting system. In Proceedings of the 22nd acm sigkdd international conference on knowledge discovery and data mining (pp. 785-794).

Incorporated Regression models:

2.6.2.1. Linear Regressio

- 2.6.2.2. Lasso Regression
- 2.6.2.3. Ridge Regression
- 2.6.2.4. ElasticNet
- 2.6.2.5. Bayesian Ridge Regression [34]

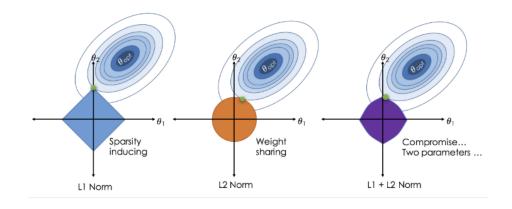


Fig. ElasticNet [43]



[34]

[43]

Incorporated Regression models:

2.6.2.6. Adaboost

2.6.2.7. ARD Regression

2.6.2.8. Decision Tree

2.6.2.9. Extra Trees

2.6.2.10. Random Forest

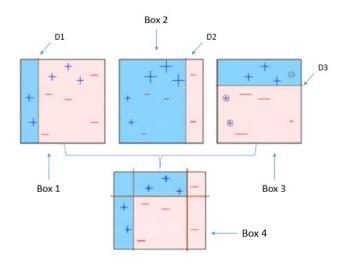


Fig. Adaboost [44]



Incorporated Regression models:

2.6.2.11.	Gaussian	Process	[35]
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- 2.6.2.12. Hist Gradient Boosting
- 2.6.2.13. k Nearest Neighbors
- **2.6.2.14.** Linear Support Vector Machine (SVM)
- 2.6.2.15. Multi-Layer Perceptron (MLP)

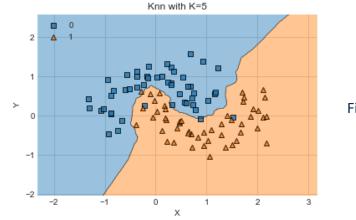


Fig. kNN [45]



[35]

[45]

Incorporated Regression models:

2.6.2.16. SGD

2.6.1.17. Light Gradient Boosting Machine (LightGBM) [36]

2.6.1.18. Extreme Gradient Boosting (XGBoost) [37]

2.6.1.19. Generalized Additive Models (GAM) [38]

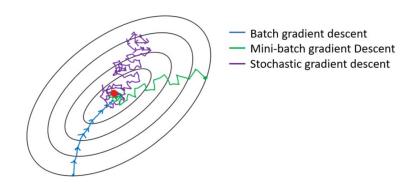


Fig. Different Gradient Descent [46]



[36]

^[37] Chen, T., & Guestrin, C. (2016, August). Xgboost: A scalable tree boosting system. In Proceedings of the 22nd acm sigkdd international conference on knowledge discovery and data mining (pp. 785-794).

^[38] Servén D., Brummitt C. (2018). pyGAM: Generalized Additive Models in Python. Zenodo. DOI: 10.5281/zenodo.1208723

2.7. Model Selection & Hyperparameter Optimization



To connect all preprocessing methods and models with hyperparameter space, we use **ray.tune** [47] for model selection and hyperparameter optimization.

ray.tune is a scalable Python package to conduct experiments on hyperparameter tuning with all common ML model structures (scikitlearn [39], TensorFlow [48], PyTorch [49], ...) with search algorithms like Optuna [50], HyperOpt [51], ...

Abadi, M., Barham, P., Chen, J., Chen, J., Chen, J., Davis, A., Dean, J., ... & Zheng, X. (2016). {TensorFlow}: a system for {Large-Scale} machine learning. In 12th USENIX symposium on operating systems design and implementation (OSDI 16) (pp. 265-283).

Paszke, A., Gross, S., Massa, F., Lerer, A., Bradbury, J., Chanan, G., ... & Chintala, S. (2019). Pytorch: An imperative style, high-performance deep learning library. Advances in neural information processing systems, 32.

Akiba, T., Sano, S., Yanase, T., Ohta, T., & Koyama, M. (2019, July). Optuna: A next-generation hyperparameter optimization framework. In Proceedings of the 25th ACM SIGKDD international conference on knowledge discovery & data mining (pp. 2623-2631)

2.7. Model Selection & Hyperparameter Optimization

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TabularObjective Ofc002e1			tabular classification	4	2.32355		fitted	-0.760684
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TabularObjective 1035621f	TERMINATED		tabular classification	4	1.58028	I ODA	fitted	-0.623932
TabularObjective 105bf1b1	TERMINATED		tabular classification	4	2.67778	LDA	fitted	-0.846154
TabularObjective 10f02794	TERMINATED		tabular classification	4	8.94002	RandomForest	fitted	-0.57265
TabularObjective 13e17e33	TERMINATED		tabular classification	4	162.87	GradientBoostingClassifier	fitted	-0.632479
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TabularObjective 1513c554	TERMINATED		tabular classification	4	3.80287	MLPClassifier	fitted	-0.794872
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TabularObjective 20f36988	TERMINATED		tabular classification	4	2.55617	LogisticRegression	fitted	-0.794872
TabularObjective 215a8d15	TERMINATED	192.168.1.89:13259	tabular classification	4	3.24688	PassiveAggressive	fitted	-0.752137
TabularObjective 22b3cf74	TERMINATED	192.168.1.89:13262	tabular classification	4	2.40195	SGD	fitted	-0.649573
TabularObjective 232c3cae	TERMINATED	192.168.1.89:13255	tabular classification	4	84.4309	KNearestNeighborsClassifier	fitted	-0.649573
TabularObjective 2372f615	TERMINATED	192.168.1.89:13266	tabular classification	4	2.80615	LogisticRegression	fitted	-0.811966
TabularObjective 23c81af2	TERMINATED	192.168.1.89:13262	tabular classification	4	2.77573	LDA	fitted	-0.615385
TabularObjective 25128f10	TERMINATED	192.168.1.89:13259	tabular classification	4	5.02668	LogisticRegression	fitted	-0.846154
TabularObjective 2598d4a8	TERMINATED	192.168.1.89:13266	tabular classification	4	61.6135	LogisticRegression	fitted	-0.82906
TabularObjective 26030ca9	TERMINATED	192.168.1.89:13262	tabular classification	4	8.97118	AdaboostClassifier	fitted	-0.777778
TabularObjective 274d7be4	TERMINATED	192.168.1.89:13259	tabular classification	4	1.81201	HistGradientBoostingClassifier	fitted	-0.846154
TabularObjective_29442fec	TERMINATED	192.168.1.89:13259	tabular_classification	4	4.62255	BernoulliNB	fitted	-0.717949
TabularObjective_2a736e7a	TERMINATED	192.168.1.89:13262	tabular_classification	4	2.88022	Libsvm_svc	fitted	-0.632479
TabularObjective_2cbd7ab9	TERMINATED		tabular_classification	4	2.93541	LogisticRegression	fitted	-0.846154
TabularObjective_2d461883	TERMINATED	192.168.1.89:13262	tabular_classification	4	11.6529	RandomForest	fitted	-0.846154
TabularObjective_2e985b00	TERMINATED	192.168.1.89:13259	tabular_classification	4	3.7879	GradientBoostingClassifier	fitted	-0.735043
TabularObjective_2f669952	TERMINATED	192.168.1.89:13259	tabular_classification	4	60.0609	QDA	fitted	-0.794872
TabularObjective_31b73aac	TERMINATED	192.168.1.89:13262	tabular_classification	4	5.8072	LogisticRegression	fitted	-0.777778
TabularObjective_35c6ead9	TERMINATED	192.168.1.89:13262	tabular_classification	4	1.53908	SGD	fitted	-0.837607
TabularObjective 39432256	TERMINATER	192.168.1.89:13262	tabular classification	4	2.51557	PassiveAggressive	 fitted	-0.709402

Fig. Store evaluation experiments

Fig. Report training process



2.7. Model Selection & Hyperparameter Optimization

```
For pipeline 1:
Optimal encoding method is: DataEncoding
Optimal encoding hyperparameters:{}

Optimal imputation method is: no_processing
Optimal imputation hyperparameters:{}

Optimal balancing method is: EditedNearestNeighbor
Optimal balancing hyperparameters:{'imbalance_threshold': 0.9941343235473185, 'k': 1}

Optimal scaling method is: MinMaxScale
Optimal scaling hyperparameters:{}

Optimal feature selection method is: no_processing
Optimal feature selection hyperparameters:{}

Optimal classification model is: RandomForest
Optimal classification hyperparameters:{'bootstrap': True, 'criterion': 'entropy', 'max_depth': None, 'max_features': 0.5700333538264852, 'max_leaf_nodes': None, 'min_impurity_decrease': 0.0, 'min_samples_leaf': 19, 'min_samples_split': 18, 'min_weight_fraction_leaf': 0.0}
```

Fig. Record optimal setting for checking



Fig. Store trained pipelines



2.7.1. Model Ensemble

To fight with data imbalance, model ensemble is another common solution, which is included in the pipeline.

Three commonly-used model ensembles are included:

1. Stacking

Models are trained parallelly on all train sets, but predictions are weighted as final prediction.

2. Bagging

Models are trained on subsets of train sets, and weighted predictions as final prediction.

3. Boosting

Models are trained on error of past models, and all predictions summed as final prediction.



3. Experiments

3.1. Heart Failure Prediction (Classification)



3. Experiments

3.2. Insurance Premium Prediction (Regression)



4. Summary & Future

Summary:

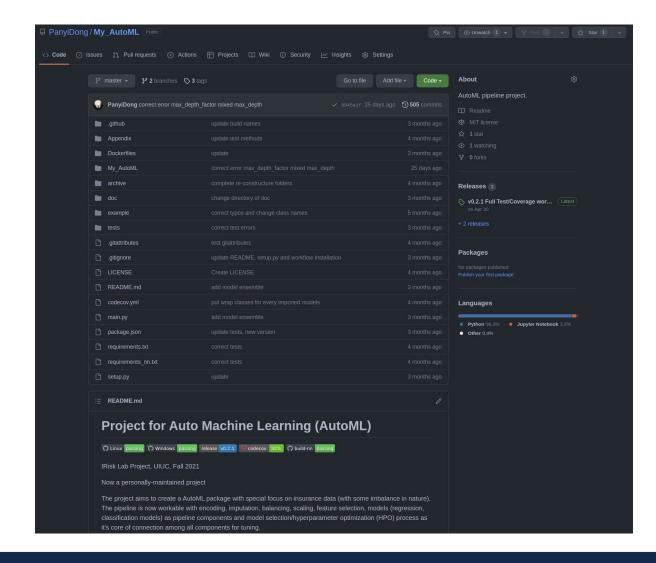
- (1) Provide a workable pipeline/framework for AutoML tasks.
- (2) **Performance** and **efficiency** of the pipeline for small datasets are at acceptable level.
- (3) For further improvement on accuracy, **increase the time budget** to allow more search & evaluations; or use current results as **baseline** to limit further search space.

Future:

- (1) Modify the search space to allow faster training; Develop/Apply better search algorithm;
- (2) Find an applicable Neural Architecture Search (NAS) algorithm and hyperparameter optimization algorithm to expand allowed tasks.
- (3) AutoML usually is time-consuming, computational-expansive, thus, train on large datasets are not feasible, which limits its applications. Apply Few-shot, One-shot idea to improve efficiency.



All code files, report and presentations are available at: https://github.com/PanyiDong/My AutoML.git



Tutorials on installment, usage are all available at the page.



Thanks!



Questions

