

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]

AutoML is an active research topic, where problems like efficiency, search algorithms are all in development.



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



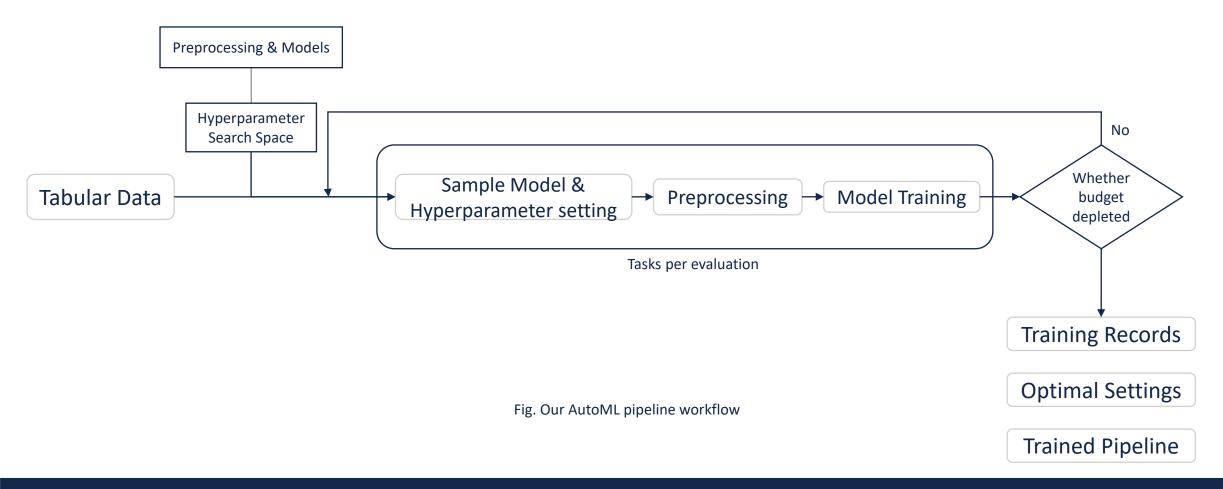
2. Components & Pipline

- 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

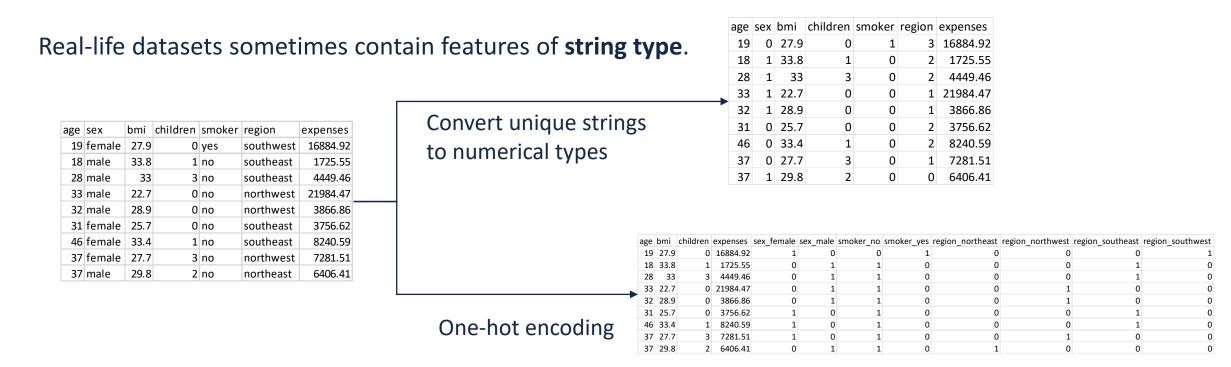


2. Components & Pipeline





2.1. Data Encoding



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



2.2. Data Imputation

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, ...



2.3. Data Balancing

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) ...

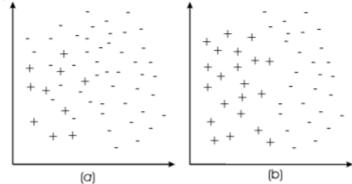


Fig. Spatial illustration of unbalanced datasets (a) and balanced datasets (b). [12]

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
- 2.4.2. Normalize
- 2.4.3. Robust Scaling
- 2.4.4. Min-Max Scaling
- 2.4.5. Power Transformer
- 2.4.6. Winsorization



2.5. Feature Selection

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.



2.6.1. Classification Models

Incorporated Classification models:

2.6.1.1. **Linear Models**

Logistic Regression, Stochastic Gradient Descent, Generalized Additive Models (GAM) [38]

2.6.1.2. **Tree Models**

Fig. Random Forest [41] Decision Tree, Extra Trees, Random Forest, Adaboost [28], Hist Gradient Boosting, Light Gradient Boosting Machine (LightGBM) [36], Extreme Gradient Boosting (XGBoost) [37]

2.6.1.3. **Nearest Neighbors**

K Nearest Neighbors

2.6.1.4. **Support Vector Machine**

Linear SVM [30], Kernel SVM [31]

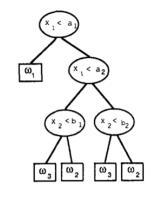
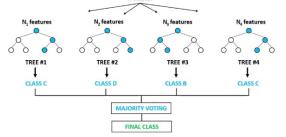
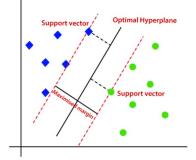


Fig. Decision Tree Split [29]







2.6.1. Classification Models

Incorporated Classification models:

2.6.1.5. Naïve Bayes (NB)

Bernoulli NB, Gaussian NB, Multinomial NB

2.6.1.6. Discriminant Analysis

Linear Discriminant Analysis (LDA), Quadratic Discriminant Analysis (QDA)

2.6.1.7. Others

Multi-Layer Perception (MLP), Passive Aggressive (PA)

Fig. Illustration of LDA

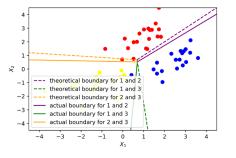


Fig. Illustration of QDA[42]

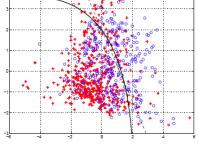


Fig. Multi-Layer Perceptron [33]

2.6.2. Regression Models

Incorporated Regression models:

2.6.2.1. Linear Models

Linear Regression, Lasso Regression, Ridge Regression, ElasticNet, Bayesian Ridge Regression [34], Adaboost, ARD Regression, SGD, Generalized Additive Models (GAM) [38]

2.6.2.2. Tree Models

Decision Tree, Extra Trees, Random Forest, Hist Gradient Boosting, Light Gradient Boosting Machine (LightGBM) [36], Extreme Gradient Boosting (XGBoost) [37]

2.6.1.3. Support Vector Machine

Linear SVM [30], Kernel SVM [31]

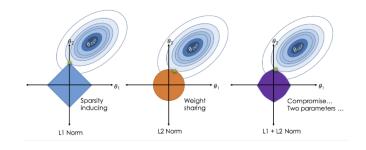
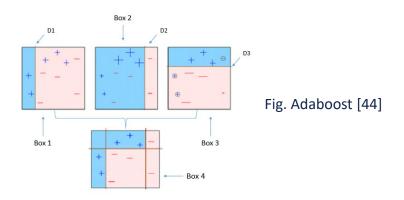


Fig. ElasticNet [43]



Servén D., Brummitt C. (2018). pyGAM: Generalized Additive Models in Python. Zenodo. <u>DOI: 10.5281/zenodo.1208723</u>

[41] https://www.freecodecamp.org/news/how-to-use-the-tree-based-algorithm-for-machine-learning/

[43] <a href="https://bowardsdatasciones.com/from-linear-regression-to-ridge-regression-the-lasso-and-the-elas-in-decamp-regression-to-ridge-regression-the-lasso-and-the-elas-in-decamp-regression-to-ridge-regression-the-lasso-and-the-elas-in-decamp-regression-to-ridge-regression-the-lasso-and-the-elas-in-decamp-regression-to-ridge-regression-the-lasso-and-the-elas-in-decamp-regression-the-regression-the-regression-the-lasso-and-the-elas-in-decamp-regression-the-regression-the-regression-the-lasso-and-the-elas-in-decamp-regression-the-regression-t

https://towardsdatascience.com/from-linear-regression-to-ridge-regression-the-lasso-and-the-elastic-net-4eaecaf5f7e6

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).

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).

2.6.2. Regression Models

Incorporated Regression models:

2.6.2.4. Nearest NeighborsK Nearest Neighbors

2.6.2.5. Others

Gaussian Process [35], Multi-Layer Perception (MLP)

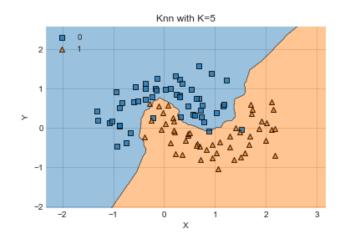


Fig. kNN [45]

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], ...

[49]

Abadi, M., Barham, P., Chen, J., Chen, J., Chen, J., 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).

Bergstra, J., Yamins, D., & Cox, D. D. (2013, June). Hyperopt: A python library for optimizing the hyperparameters of machine learning algorithms. In Proceedings of the 12th Python in science conference (Vol. 13, p. 20).

2.7. Model Selection & Hyperparameter Optimization

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TabularObjective Ofdaf193	TERMINATED		tabular classification	4	3.57492	BernoulliNB	fitted	-0.589744
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TabularObjective 1513c554	TERMINATED		tabular classification	4	3.80287	MLPClassifier	fitted	-0.794872
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TabularObjective 1944fd72	TERMINATED	192.168.1.89:13253	tabular classification	4	5.22084	HistGradientBoostingClassifier	fitted	-0.777778
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TabularObjective 1b71772e	TERMINATED		tabular classification	4	4.5688	LogisticRegression	fitted	-0.846154
TabularObjective 1ba85298	TERMINATED		tabular classification	4	158.035	LibLinear SVC	fitted	-0.589744
TabularObjective 1cfb6a4a	TERMINATED	192.168.1.89:13266	tabular classification	4	6.16606	LDA	fitted	-0.803419
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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. Live Experiments

3.1. Heart Failure Prediction (Classification)

- (1) One-line command job
- (2) Package-style usage



4. Summary & Future

Summary:

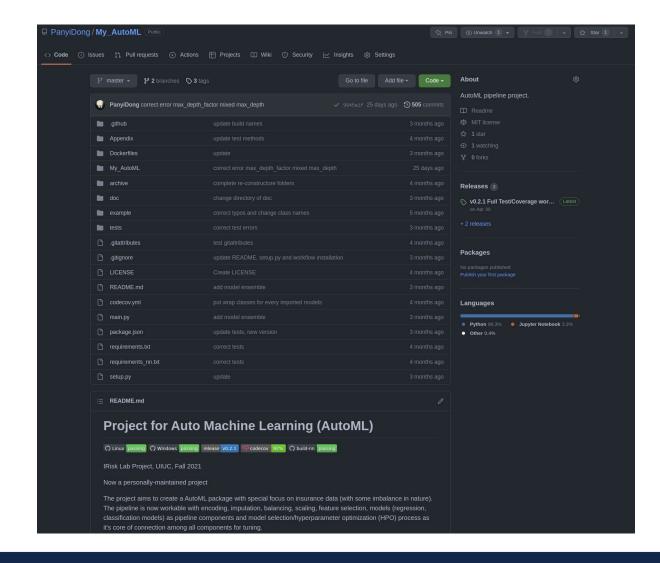
- (1) Provide a workable pipeline/framework for AutoML tasks.
- (2) **Performance** and **efficiency** of the pipeline for small datasets are at acceptable level.
- (3) For further improvement on accuracy, **increase the time budget** to allow more search & evaluations; or use current results as **baseline**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

