Automated Machine Learning (AutoML) in Insurance

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1. Introduction to AutoML

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) ….

Fig. Self-Driving Cars [2]

For Insurance:

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

[1] Mitchell, T. M., & Mitchell, T. M. (1997). *Machine learning* (Vol. 1, No. 9). New York: McGraw-hill.
[2] https://www.imeche.org/news/news-article/webinar-autonomous-vehicles---the-challenges-of-automated-driving

1. Introduction to AutoML

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.

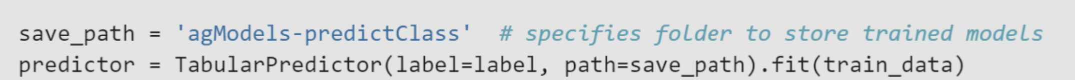
Furthermore, industrial datasets usually are not well-formatted or well-organized, and problems like **missing values**, **irrelevant features**, **imbalance distributions** exists.

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

1. Introduction to AutoML

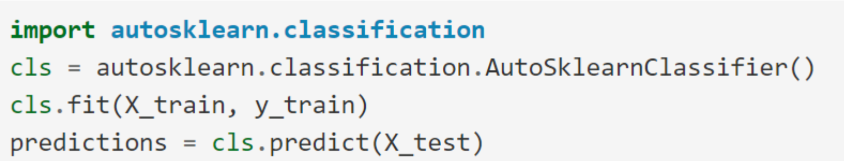
Automated Machine Learning (AutoML) is one of the solutions.

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]



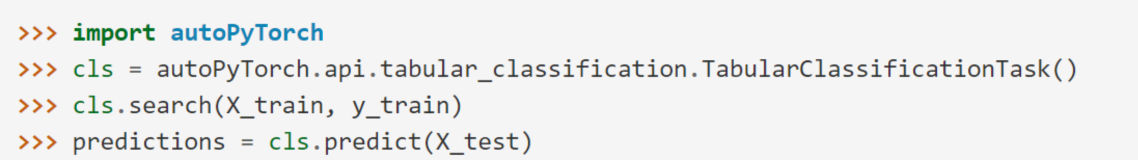
```
save_path = 'agModels-predictClass'  # specifies folder to store trained models
predictor = TabularPredictor(label=label, path=save_path).fit(train_data)
```

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).
[4] https://auto.gluon.ai/stable/index.html
[5] https://automl.github.io/auto-sklearn/master/
[6] https://automl.github.io/Auto-PyTorch/development/

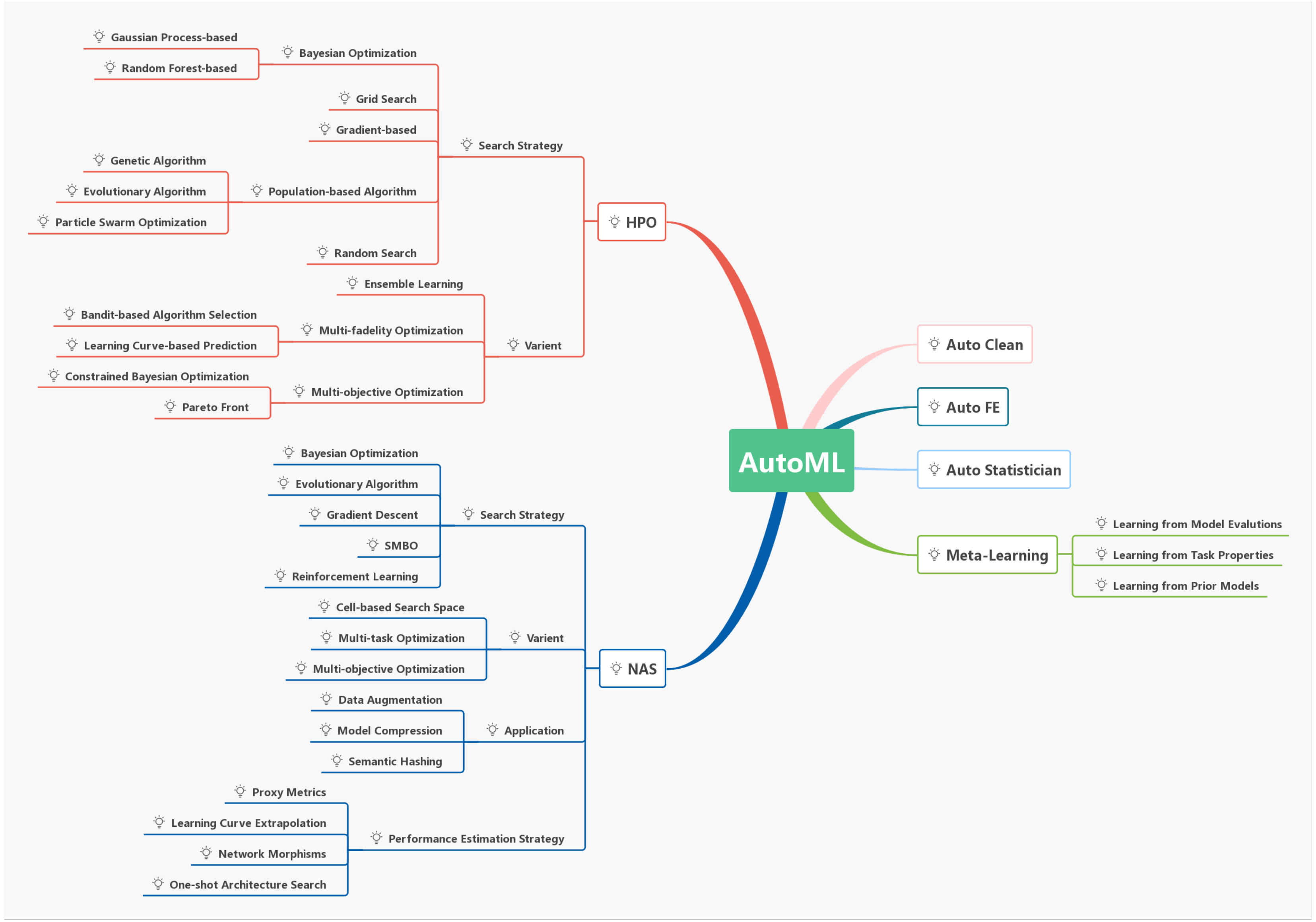


Fig. AutoML research mainstream [7]

[7] https://github.com/hibayesian/awesome-automl-papers/blob/master/resources/automl.png

1. Introduction to AutoML

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

1. Introduction to AutoML

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

Preprocessing

6. Classification/Regression Models
7. Model Selection and Hyperparameter Optimization

2. Components & Pipeline

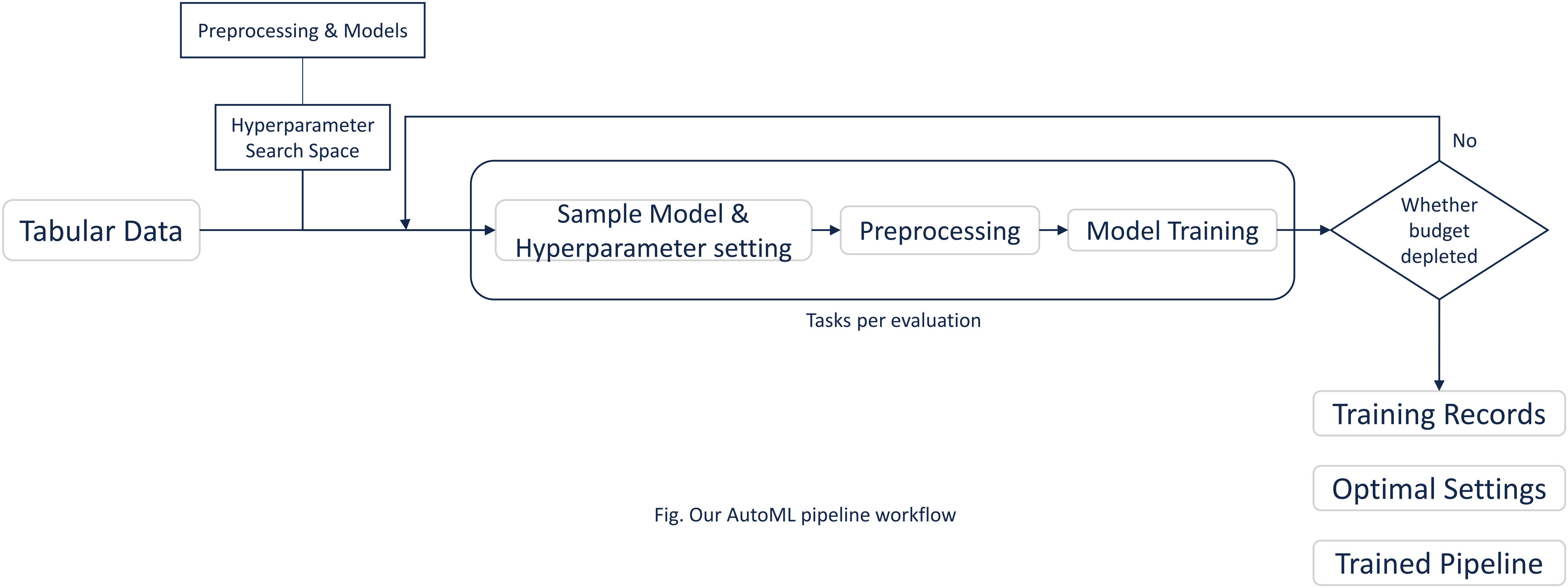
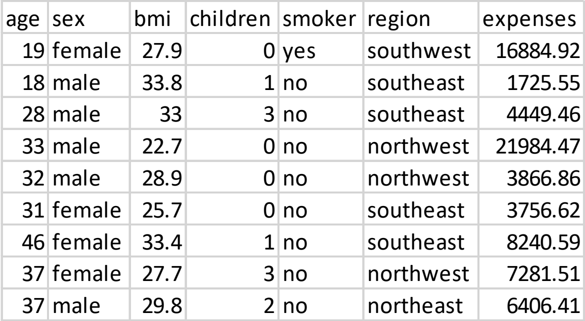


Fig. Our AutoML pipeline workflow

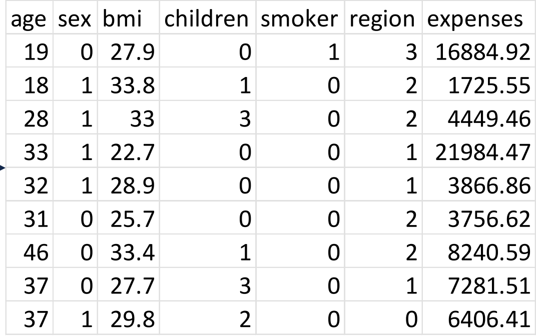
2.1. Data Encoding

Real-life datasets sometimes contain features of **string type**.



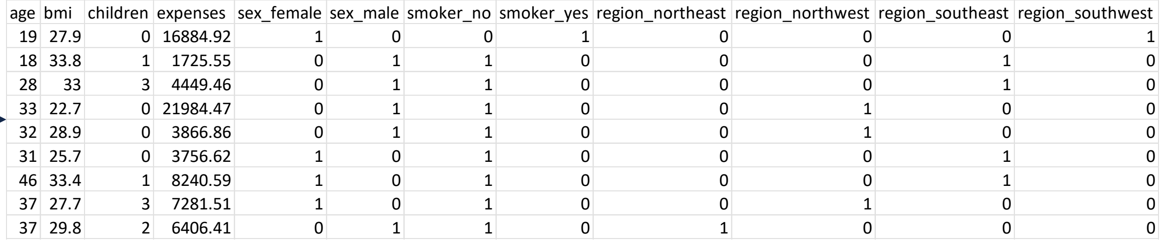
age	sex	bmi	children	smoker	region	expenses
19	female	27.9	0	yes	southwest	16884.92
18	male	33.8	1	no	southeast	1725.55
28	male	33	3	no	southeast	4449.46
33	male	22.7	0	no	northwest	21984.47
32	male	28.9	0	no	northwest	3866.86
31	female	25.7	0	no	southeast	3756.62
46	female	33.4	1	no	southeast	8240.59
37	female	27.7	3	no	northwest	7281.51
37	male	29.8	2	no	northeast	6406.41

Convert unique strings to numerical types



age	sex	bmi	children	smoker	region	expenses
19	0	27.9	0	1	3	16884.92
18	1	33.8	1	0	2	1725.55
28	1	33	3	0	2	4449.46
33	1	22.7	0	0	1	21984.47
32	1	28.9	0	0	1	3866.86
31	0	25.7	0	0	2	3756.62
46	0	33.4	1	0	2	8240.59
37	0	27.7	3	0	1	7281.51
37	1	29.8	2	0	0	6406.41

One-hot encoding



age	bmi	children	expenses	sex_female	sex_male	smoker_no	smoker_yes	region_northeast	region_northwest	region_southeast	region_southwest
19	27.9	0	16884.92	1	0	0	1	0	0	0	1
18	33.8	1	1725.55	0	1	1	0	0	0	1	0
28	33	3	4449.46	0	1	1	0	0	0	1	0
33	22.7	0	21984.47	0	1	1	0	0	1	0	0
32	28.9	0	3866.86	0	1	1	0	0	1	0	0
31	25.7	0	3756.62	1	0	1	0	0	0	1	0
46	33.4	1	8240.59	1	0	1	0	0	0	1	0
37	27.7	3	7281.51	1	0	1	0	0	1	0	0
37	29.8	2	6406.41	0	1	1	0	1	0	0	0

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, …

2.2. Data Imputation

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.

2.2. Data Imputation

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.

[8] Musil, C. M., Warner, C. B., Yobas, P. K., & Jones, S. L. (2002). A comparison of imputation techniques for handling missing data. Western journal of nursing research, 24(7), 815-829.

[9] Stekhoven, D. J., & Bühlmann, P. (2012). MissForest—non-parametric missing value imputation for mixed-type data. Bioinformatics, 28(1), 112-118.

2.2. Data Imputation

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.

[10] Azur, M. J., Stuart, E. A., Frangakis, C., & Leaf, P. J. (2011). Multiple imputation by chained equations: what is it and how does it work?. International journal of methods in psychiatric research, 20(1), 40-49.

[11] Yoon, J., Jordon, J., & Schaar, M. (2018, July). Gain: Missing data imputation using generative adversarial nets. In International conference on machine learning (pp. 5689-5698). PMLR.

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) …

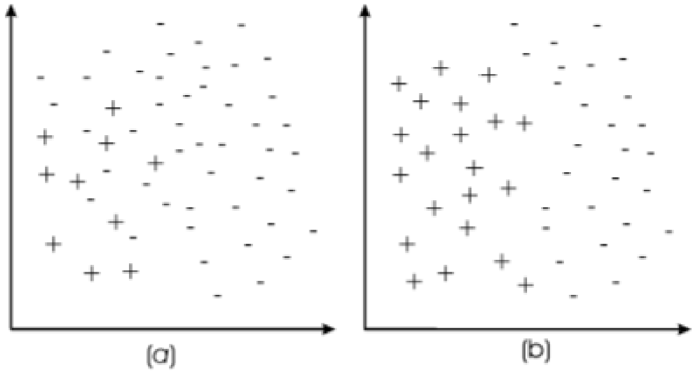


Fig. Spatial illustration of unbalanced datasets (a) and balanced datasets (b). [12]

[12] Batista, G. E., Prati, R. C., & Monard, M. C. (2004). A study of the behavior of several methods for balancing machine learning training data. ACM SIGKDD explorations newsletter, 6(1), 20-29.

2.3. Data Balancing

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.

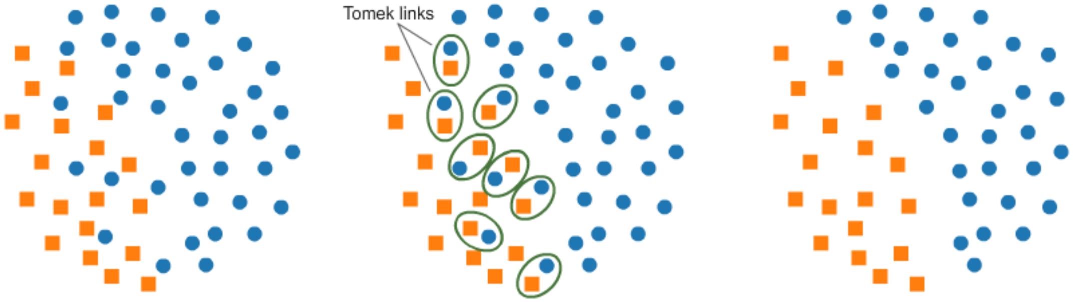


Fig. Illustration of Tomek Link [14]

[13] Tomek, I. (1976). Two modifications of CNN.

[14] https://mlwhiz.com/blog/2020/01/28/imbal/

2.3. Data Balancing

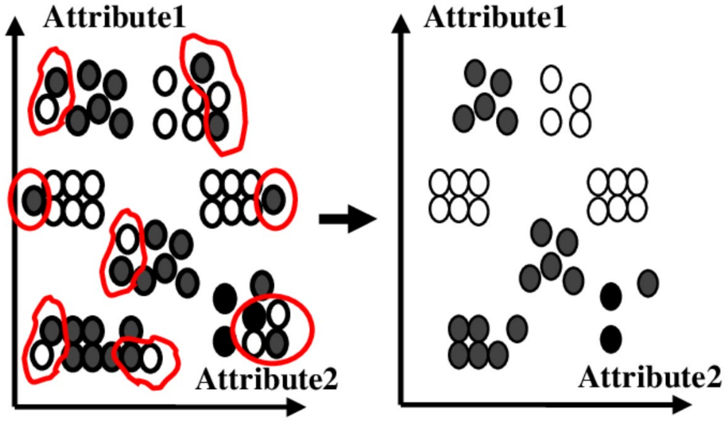


Fig. Illustration Edited Nearest Neighbor [16]

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.

2.3.5. Condensed Nearest Neighbors (CNN) [17]

An Under-Sampling method.
Select a subset of observations $\hat{E} \subseteq E$ where $\hat{E}$ can predict all observations correctly using 1-NN.

[15] Wilson, D. L. (1972). Asymptotic properties of nearest neighbor rules using edited data. IEEE Transactions on Systems, Man, and Cybernetics, (3), 408-421.
[16] https://www.researchgate.net/figure/Wilson-Editing-for-a-1-NN-Classifier_fig1_4133603
[17] Hart, P. (1968). The condensed nearest neighbor rule (corresp.). IEEE transactions on information theory, 14(3), 515-516.

2.3. Data Balancing

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.

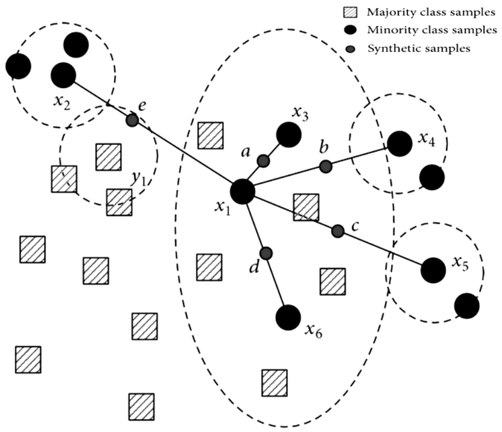


Fig. Illustration of Smote [19]

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.

[18] Chawla, N. V., Bowyer, K. W., Hall, L. O., & Kegelmeyer, W. P. (2002). SMOTE: synthetic minority over-sampling technique. Journal of artificial intelligence research, 16, 321-357.
[19] https://towardsdatascience.com/stop-using-smote-to-handle-all-your-imbalanced-data-34403399d3be

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).

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.

[20] Chandrashekar, G., & Sahin, F. (2014). A survey on feature selection methods. Computers & Electrical Engineering, 40(1), 16-28.

2.5. Feature Selection

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

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

2.5. Feature Selection

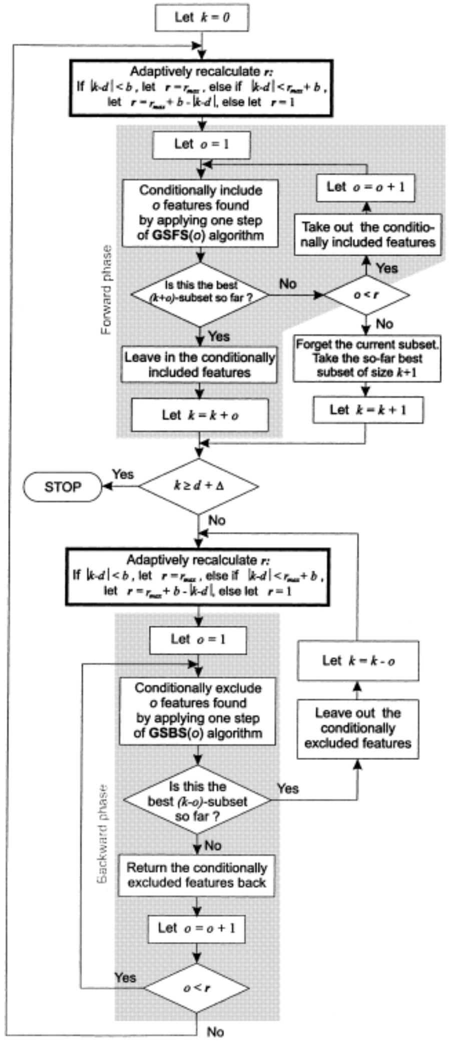
Incorporated Feature Selection methods:

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.



Let $k = 0$
Adaptively recalculate r:
If $|k-d| < b$, let $r = r_{max}$, else if $|k-d| < r_{max} + b$,
let $r = r_{max} + b - |k-d|$, else let $r = 1$
Forward phase
Let $o = 1$
Conditionally include o features found by applying one step of **GSFS**(o) algorithm
Is this the best $(k+o)$-subset so far ?
No
$o < r$
Yes
Take out the conditionally included features
Let $o = o + 1$
No
Forget the current subset. Take the so-far best subset of size $k+1$
Let $k = k + 1$
Yes
Leave in the conditionally included features
Let $k = k + o$
STOP
Yes
$k \geq d + \Delta$
No
Adaptively recalculate r:
If $|k-d| < b$, let $r = r_{max}$, else if $|k-d| < r_{max} + b$,
let $r = r_{max} + b - |k-d|$, else let $r = 1$
Backward phase
Let $o = 1$
Conditionally exclude o features found by applying one step of **GSBS**(o) algorithm
Is this the best $(k-o)$-subset so far ?
Yes
Leave out the conditionally excluded features
Let $k = k - o$
No
Return the conditionally excluded features back
Let $o = o + 1$
Yes
$o < r$
No

Fig. Workflow of ASFFS [21]

[21] Somol, P., Pudil, P., Novovičová, J., & Paclık, P. (1999). Adaptive floating search methods in feature selection. Pattern recognition letters, 20(11-13), 1157-1163.

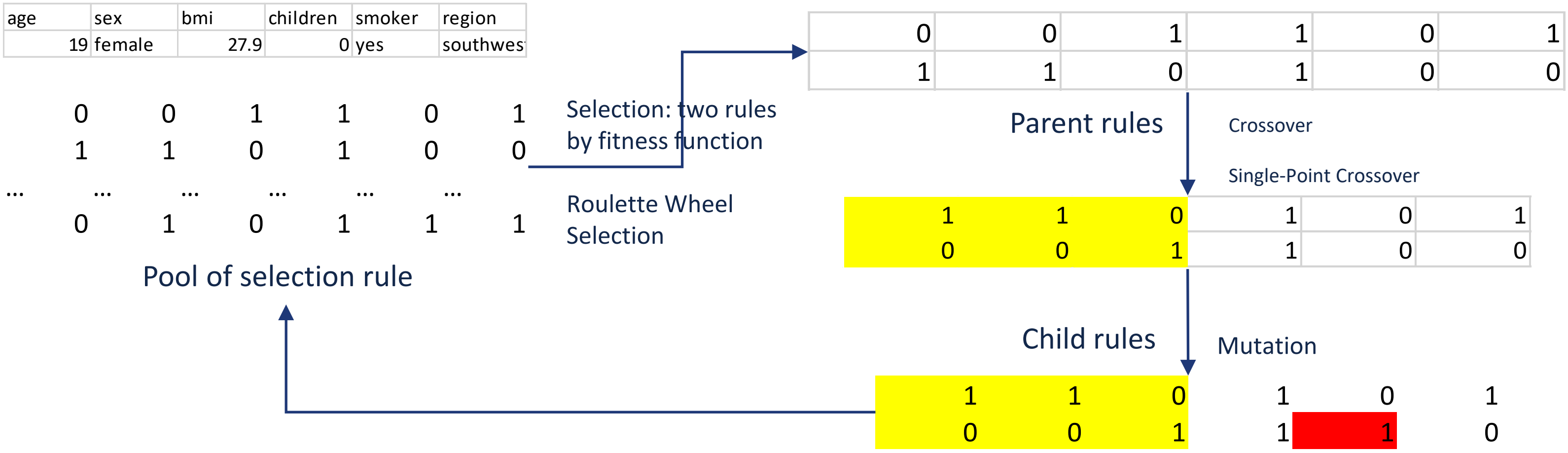
2.5. Feature Selection

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.



age	sex	bmi	children	smoker	region
19	female	27.9	0	yes	southwes

0	0	1	1	0	1
1	1	0	1	0	0
…	…	…	…	…	…
0	1	0	1	1	1

Pool of selection rule

Selection: two rules by fitness function

Roulette Wheel Selection

0	0	1	1	0	1
1	1	0	1	0	0

Parent rules

Crossover

Single-Point Crossover

1	1	0	1	0	1
0	0	1	1	0	0

Child rules

Mutation

1	1	0	1	0	1
0	0	1	1	1	0

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

[22] Tan, F., Fu, X., Zhang, Y., & Bourgeois, A. G. (2008). A genetic algorithm-based method for feature subset selection. Soft Computing, 12(2), 111-120.

2.5. Feature 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.

[23] Liu, Y., Tang, F., & Zeng, Z. (2014). Feature selection based on dependency margin. IEEE Transactions on Cybernetics, 45(6), 1209-1221.
[24] 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.
[26] Lall, S., Sinha, D., Ghosh, A., Sengupta, D., & Bandyopadhyay, S. (2021). Stable feature selection using copula based mutual information. Pattern Recognition, 112, 107697.
[27] Lall, S., & Bandyopadhyay, S. (2019, September). An l1-Norm regularized copula based feature selection. In Proceedings of the 2019 3rd International Symposium on Computer Science and Intelligent Control (pp. 1-6).

2.6.1. Classification Models

Incorporated Classification models:

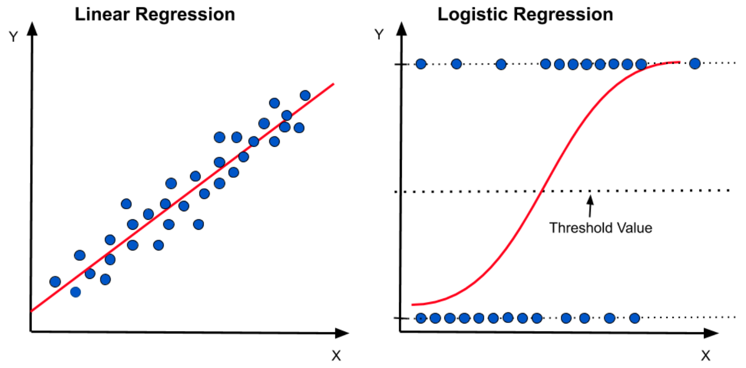


Fig. Linear Regression vs Logistic Regression [53]

2.6.1.1. Logistic Regression

2.6.1.2. Adaboost [28]

Adaboost takes the structure of ensemble, each weak learner is trained on the same data with adjusted weights (heavier weight for wrong predictions).

2.6.1.3. Hist Gradient Boosting

Histogram-based Gradient Boosting is a specific structure of Gradient Boosting, discretization continuous values into ranges of bins to speed up.

[28] Hastie, T., Rosset, S., Zhu, J. & Zou, H. Multi-class adaboost. Statistics and its Interface 2, 349–360 (2009).
[53] https://ai.plainenglish.io/why-is-logistic-regression-called-regression-if-it-is-a-classification-algorithm-9c2a166e7b74

2.6.1. Classification Models

Incorporated Classification models:

2.6.1.4. Linear Support Vector Machine (SVM) [30]

2.6.1.5. Kernel Support Vector Machine (SVM) [31]

One of the most popular model architecture in early 2000s.

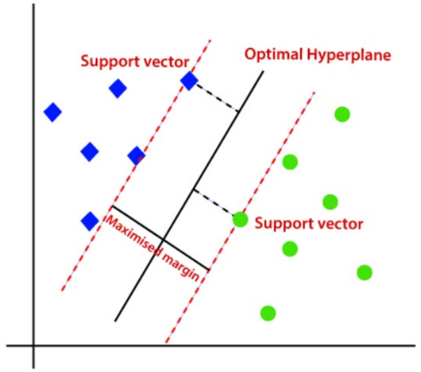


Fig. Support Vector Machine [32]

[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).
[31] 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

2.6.1. Classification Models

Incorporated Classification models:

2.6.1.6. Decision Tree

2.6.1.7. Extra Trees

An ensemble of extremely **randomized** decision trees.
Each trained on subset of samples.

2.6.1.8. Random Forest

An ensemble of extremely decision trees.
Each trained on subset of samples.

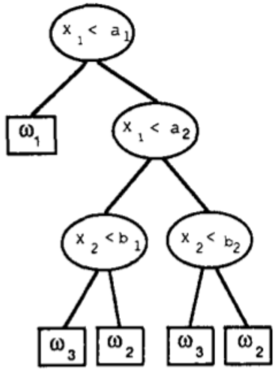


Fig. Decision Tree Split [29]

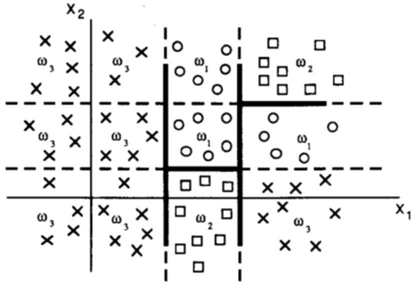


Fig. Split On Data Points [29]

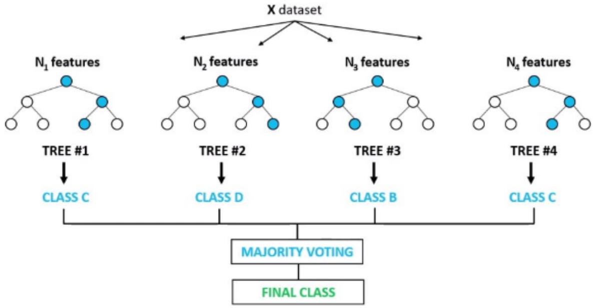


Fig. Random Forest [41]

[29] Safavian, S. R. & Landgrebe, D. A survey of decision tree classifier methodology. IEEE transactions on systems, man, and cybernetics 21, 660–674 (1991).
[41] https://www.freecodecamp.org/news/how-to-use-the-tree-based-algorithm-for-machine-learning/

2.6.1. Classification Models

Incorporated Classification models:

2.6.1.9. K Nearest Neighbors

A distance-based method, similarly behavior should within closest range.

2.6.1.10. SGD

Regularized linear models with Stochastic Gradient Descent optimization.

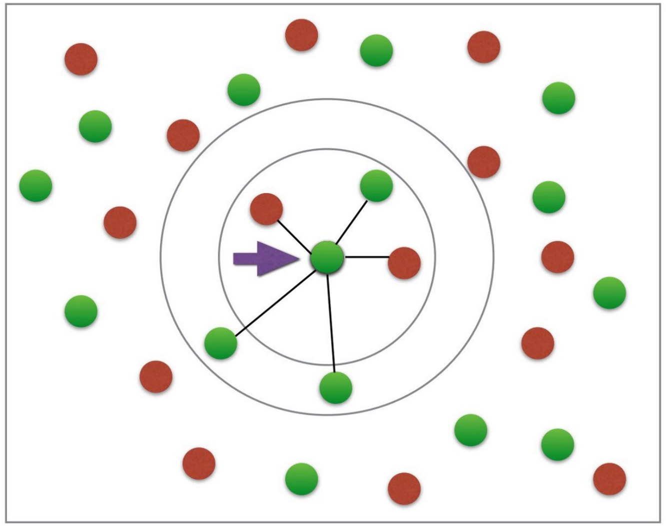


Fig. K Nearest Neighbors [54]

[29] Safavian, S. R. & Landgrebe, D. A survey of decision tree classifier methodology. IEEE transactions on systems, man, and cybernetics 21, 660–674 (1991).
[41] https://www.freecodecamp.org/news/how-to-use-the-tree-based-algorithm-for-machine-learning/

2.6.1. Classification Models

Incorporated Classification models:

2.6.1.11. Linear Discriminant Analysis (LDA)

2.6.1.12. Quadratic Discriminant Analysis (QDA)

Linear/Quadratic decision boundary by optimizing the distance of observations to the boundary.

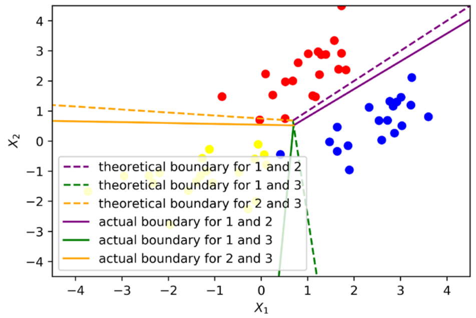


Fig. Linear Discriminant Analysis

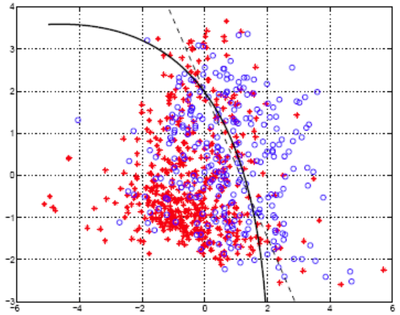


Fig. Quadratic Discriminant Analysis [42]

[42] https://online.stat.psu.edu/stat508/book/export/html/696

2.6.1. Classification Models

Incorporated Classification models:

2.6.1.13. Bernoulli Naïve Bayes

2.6.1.14. Gaussian Naïve Bayes

2.6.1.15. Multinomial Naïve Bayes

Probabilistic classifiers utilizing Bayes rule

[42] https://online.stat.psu.edu/stat508/book/export/html/696

2.6.1. Classification Models

Incorporated Classification models:

2.6.1.16. Multi-Layer Perception (MLP)

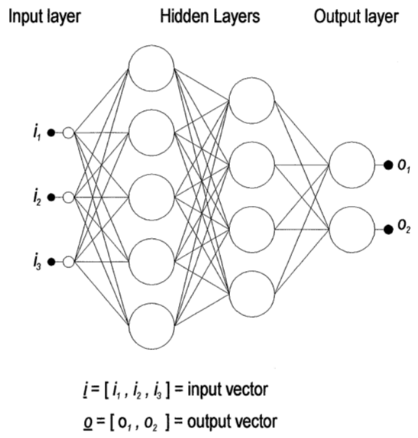
2.6.1.17. Passive Aggressive

Online learning algorithm that only updates when model is wrong.

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]



Input layer
Hidden Layers
Output layer
i_1
i_2
i_3
o_1
o_2
$\underline{i} = [\, i_1 , i_2 , i_3 \,]$ = input vector
$\underline{o} = [\, o_1 , o_2 \,]$ = output vector

Fig. Multi-Layer Perceptron [33]

[33] Gardner, M. W. & Dorling, S. Artificial neural networks (the multilayer perceptron)—a review of applications in the atmospheric sciences. Atmospheric environment 32, 2627–2636 (1998).

[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.

[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

2.6.2. Regression Models

Incorporated Regression models:

2.6.2.1. Linear Regression

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]

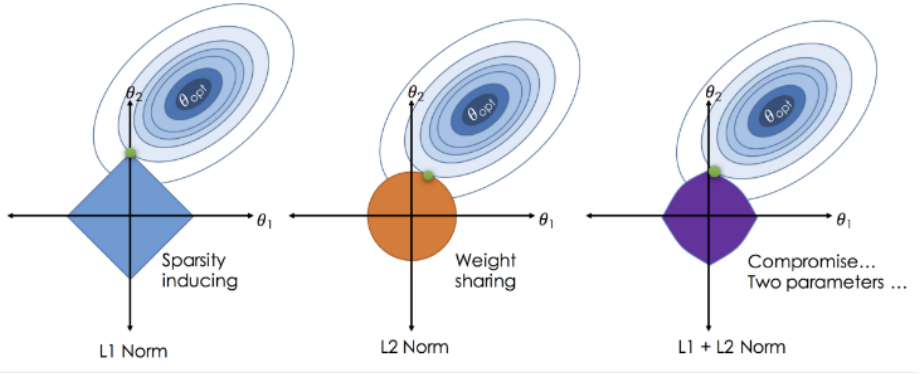


Fig. ElasticNet [43]

[34] Wilhelm, F. The idea behind automatic relevance determination and bayesian interpolation. https://www.youtube.com/watch?v=2gT-Q0NZzoE (2016).
[43] https://towardsdatascience.com/from-linear-regression-to-ridge-regression-the-lasso-and-the-elastic-net-4eaecaf5f7e6

2.6.2. Regression Models

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**

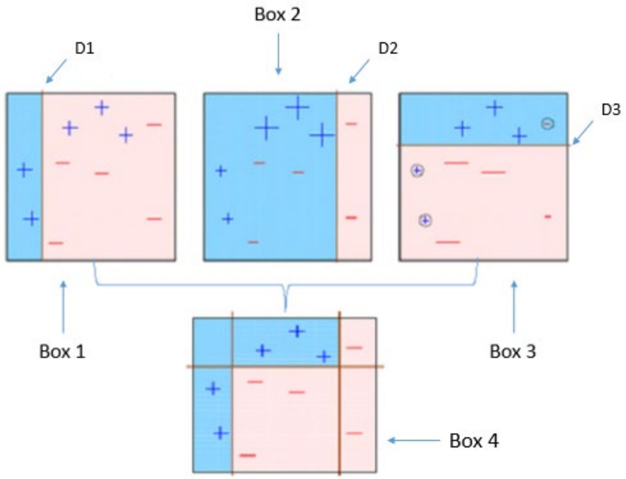


Fig. Adaboost [44]

[44] https://towardsdatascience.com/understanding-adaboost-2f94f22d5bfe

2.6.2. Regression Models

Incorporated Regression models:

2.6.2.11. Gaussian Process [35]

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)

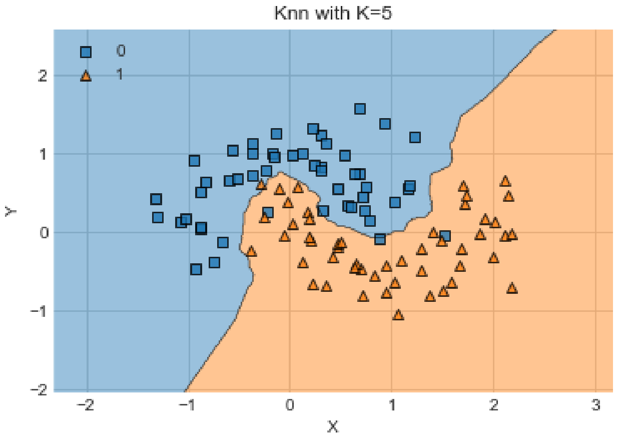


Fig. kNN [45]

[35] Wang, J. An intuitive tutorial to gaussian processes regression. arXiv preprint arXiv:2009.10862 (2020).

[45] https://towardsdatascience.com/knn-visualization-in-just-13-lines-of-code-32820d72c6b6

2.6.2. Regression Models

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]**

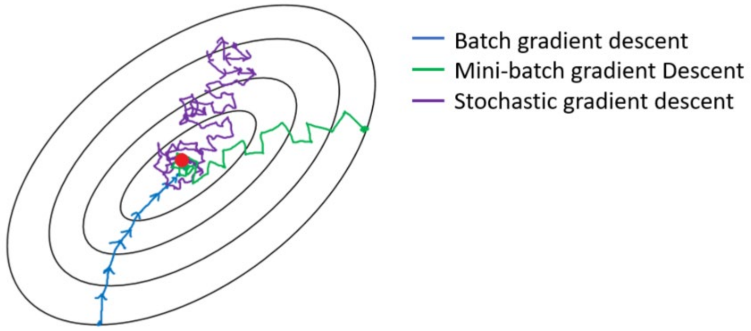


Fig. Different Gradient Descent [46]

[36] 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.
[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
[46] https://suniljangirblog.wordpress.com/2018/12/13/variants-of-gradient-descent/

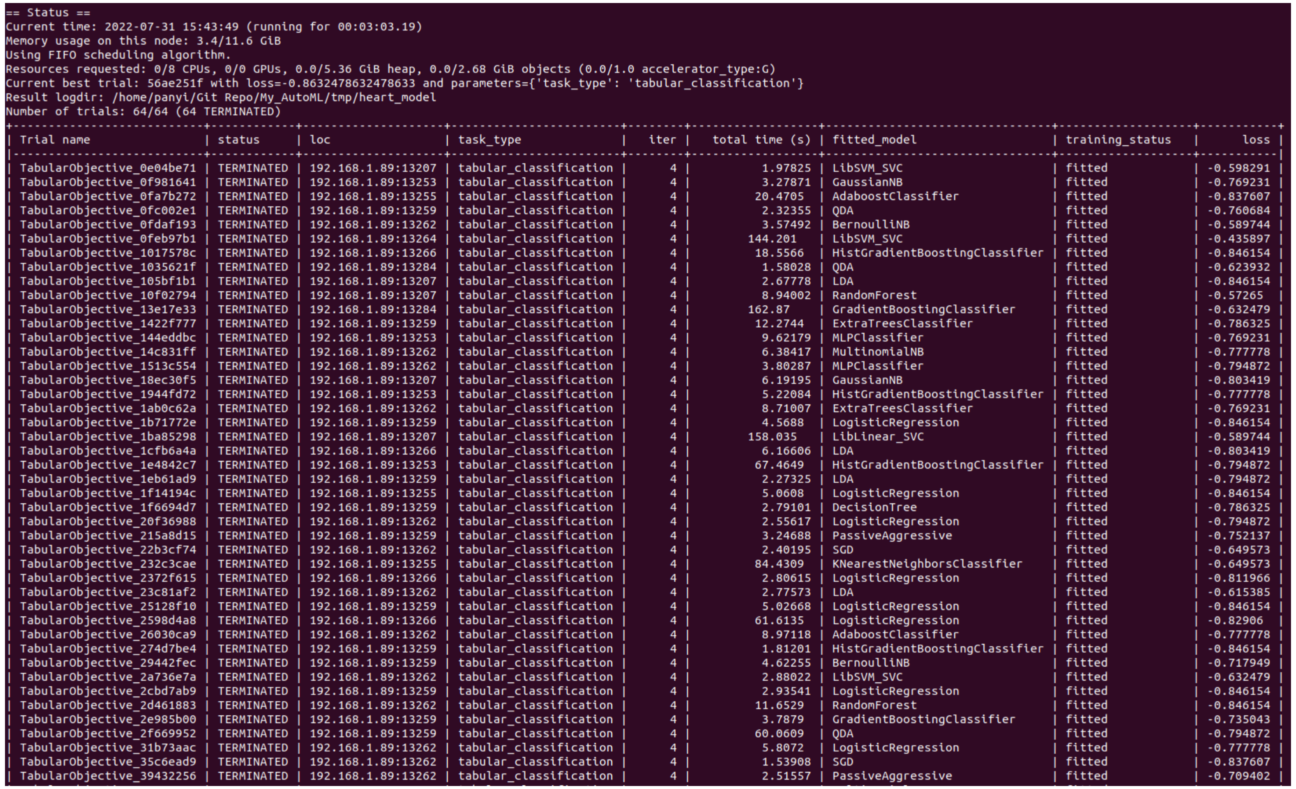
2.7. Model Selection & Hyperparameter Optimization

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 (**scikit-learn** [39], **TensorFlow** [48], **PyTorch** [49], …) with search algorithms like **Optuna** [50], **HyperOpt** [51], …

[39] Pedregosa, F., Varoquaux, G., Gramfort, A., Michel, V., Thirion, B., Grisel, O., ... & Duchesnay, E. (2011). Scikit-learn: Machine learning in Python. the Journal of machine Learning research, 12, 2825-2830.
[47] Liaw, R., Liang, E., Nishihara, R., Moritz, P., Gonzalez, J. E., & Stoica, I. (2018). Tune: A research platform for distributed model selection and training. arXiv preprint arXiv:1807.05118.
[48] Abadi, M., Barham, P., Chen, J., Chen, Z., 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).
[49] 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.
[50] 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).
[51] 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



```
== Status ==
Current time: 2022-07-31 15:43:49 (running for 00:03:03.19)
Memory usage on this node: 3.4/11.6 GiB
Using FIFO scheduling algorithm.
Resources requested: 0/8 CPUs, 0/0 GPUs, 0.0/5.36 GiB heap, 0.0/2.68 GiB objects (0.0/1.0 accelerator_type:G)
Current best trial: 56ae251f with loss=-0.8632478632478633 and parameters={'task_type': 'tabular_classification'}
Result logdir: /home/panyi/Git Repo/My_AutoML/tmp/heart_model
Number of trials: 64/64 (64 TERMINATED)
+---------------------------+------------+--------------------+------------------------+--------+----------------+--------------------------------+-----------------+-----------+
| Trial name                | status     | loc                | task_type              |   iter | total time (s) | fitted_model                   | training_status |      loss |
|---------------------------+------------+--------------------+------------------------+--------+----------------+--------------------------------+-----------------+-----------|
| TabularObjective_0e04be71 | TERMINATED | 192.168.1.89:13207 | tabular_classification |      4 |        1.97825 | LibSVM_SVC                     | fitted          | -0.598291 |
| TabularObjective_0f981641 | TERMINATED | 192.168.1.89:13253 | tabular_classification |      4 |        3.27871 | GaussianNB                     | fitted          | -0.769231 |
| TabularObjective_0fa7b272 | TERMINATED | 192.168.1.89:13255 | tabular_classification |      4 |       20.4705  | AdaboostClassifier             | fitted          | -0.837607 |
| TabularObjective_0fc002e1 | TERMINATED | 192.168.1.89:13259 | tabular_classification |      4 |        2.32355 | QDA                            | fitted          | -0.760684 |
| TabularObjective_0fdaf193 | TERMINATED | 192.168.1.89:13262 | tabular_classification |      4 |        3.57492 | BernoulliNB                    | fitted          | -0.589744 |
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| TabularObjective_1017578c | TERMINATED | 192.168.1.89:13266 | tabular_classification |      4 |       18.5566  | HistGradientBoostingClassifier | fitted          | -0.846154 |
| TabularObjective_1035621f | TERMINATED | 192.168.1.89:13284 | tabular_classification |      4 |        1.58028 | QDA                            | fitted          | -0.623932 |
| TabularObjective_105bf1b1 | TERMINATED | 192.168.1.89:13207 | tabular_classification |      4 |        2.67778 | LDA                            | fitted          | -0.846154 |
| TabularObjective_10f02794 | TERMINATED | 192.168.1.89:13207 | tabular_classification |      4 |        8.94002 | RandomForest                   | fitted          | -0.57265  |
| TabularObjective_13e17e33 | TERMINATED | 192.168.1.89:13284 | tabular_classification |      4 |      162.87    | GradientBoostingClassifier     | fitted          | -0.632479 |
| TabularObjective_1422f777 | TERMINATED | 192.168.1.89:13259 | tabular_classification |      4 |       12.2744  | ExtraTreesClassifier           | fitted          | -0.786325 |
| TabularObjective_144eddbc | TERMINATED | 192.168.1.89:13253 | tabular_classification |      4 |        9.62179 | MLPClassifier                  | fitted          | -0.769231 |
| TabularObjective_14c831ff | TERMINATED | 192.168.1.89:13262 | tabular_classification |      4 |        6.38417 | MultinomialNB                  | fitted          | -0.777778 |
| TabularObjective_1513c554 | TERMINATED | 192.168.1.89:13262 | tabular_classification |      4 |        3.80287 | MLPClassifier                  | fitted          | -0.794872 |
| TabularObjective_18ec30f5 | TERMINATED | 192.168.1.89:13207 | tabular_classification |      4 |        6.19195 | GaussianNB                     | fitted          | -0.803419 |
| TabularObjective_1944fd72 | TERMINATED | 192.168.1.89:13253 | tabular_classification |      4 |        5.22084 | HistGradientBoostingClassifier | fitted          | -0.777778 |
| TabularObjective_1ab0c62a | TERMINATED | 192.168.1.89:13262 | tabular_classification |      4 |        8.71007 | ExtraTreesClassifier           | fitted          | -0.769231 |
| TabularObjective_1b71772e | TERMINATED | 192.168.1.89:13259 | tabular_classification |      4 |        4.5688  | LogisticRegression             | fitted          | -0.846154 |
| TabularObjective_1ba85298 | TERMINATED | 192.168.1.89:13207 | 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 |
| TabularObjective_1e4842c7 | TERMINATED | 192.168.1.89:13253 | tabular_classification |      4 |       67.4649  | HistGradientBoostingClassifier | fitted          | -0.794872 |
| TabularObjective_1eb61ad9 | TERMINATED | 192.168.1.89:13259 | tabular_classification |      4 |        2.27325 | LDA                            | fitted          | -0.794872 |
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| TabularObjective_1f6694d7 | TERMINATED | 192.168.1.89:13259 | tabular_classification |      4 |        2.79101 | DecisionTree                   | fitted          | -0.786325 |
| TabularObjective_20f36988 | TERMINATED | 192.168.1.89:13262 | tabular_classification |      4 |        2.55617 | LogisticRegression             | fitted          | -0.794872 |
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| TabularObjective_232c3cae | TERMINATED | 192.168.1.89:13255 | tabular_classification |      4 |       84.4309  | KNearestNeighborsClassifier    | fitted          | -0.649573 |
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| TabularObjective_25128f10 | TERMINATED | 192.168.1.89:13259 | tabular_classification |      4 |        5.02668 | LogisticRegression             | fitted          | -0.846154 |
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| 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 | 192.168.1.89:13259 | 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 |
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| 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 | TERMINATED | 192.168.1.89:13262 | tabular_classification |      4 |        2.51557 | PassiveAggressive              | fitted          | -0.709402 |
```

Fig. Report training process

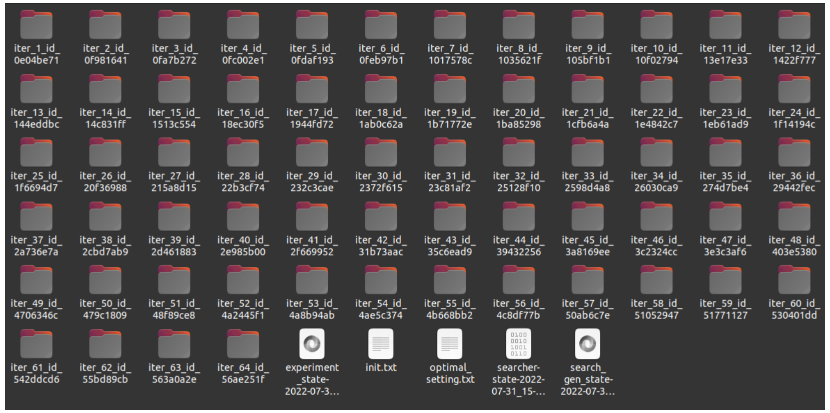
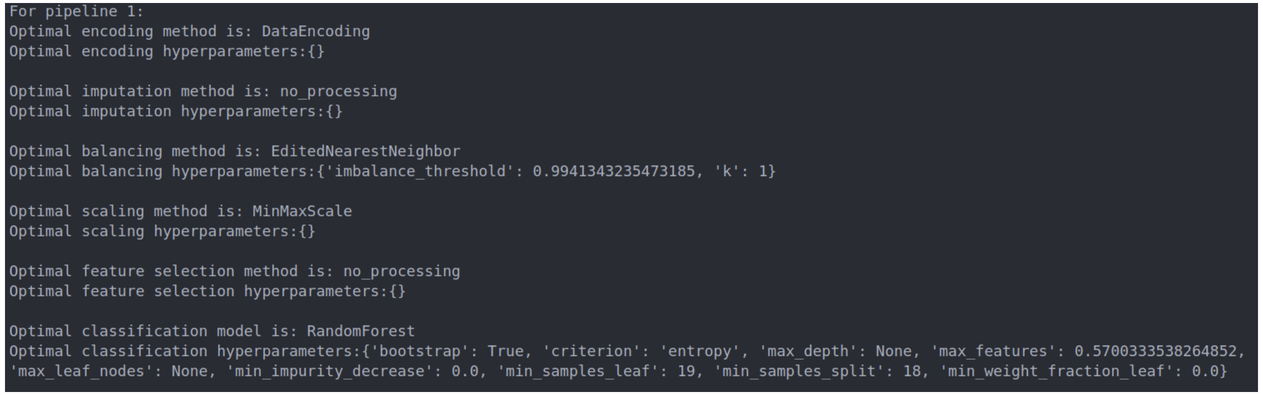


Fig. Store evaluation experiments

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

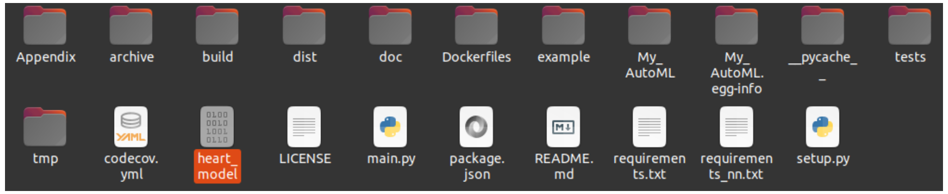


Fig. Store trained pipelines

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.

2.7.1. Model Ensemble

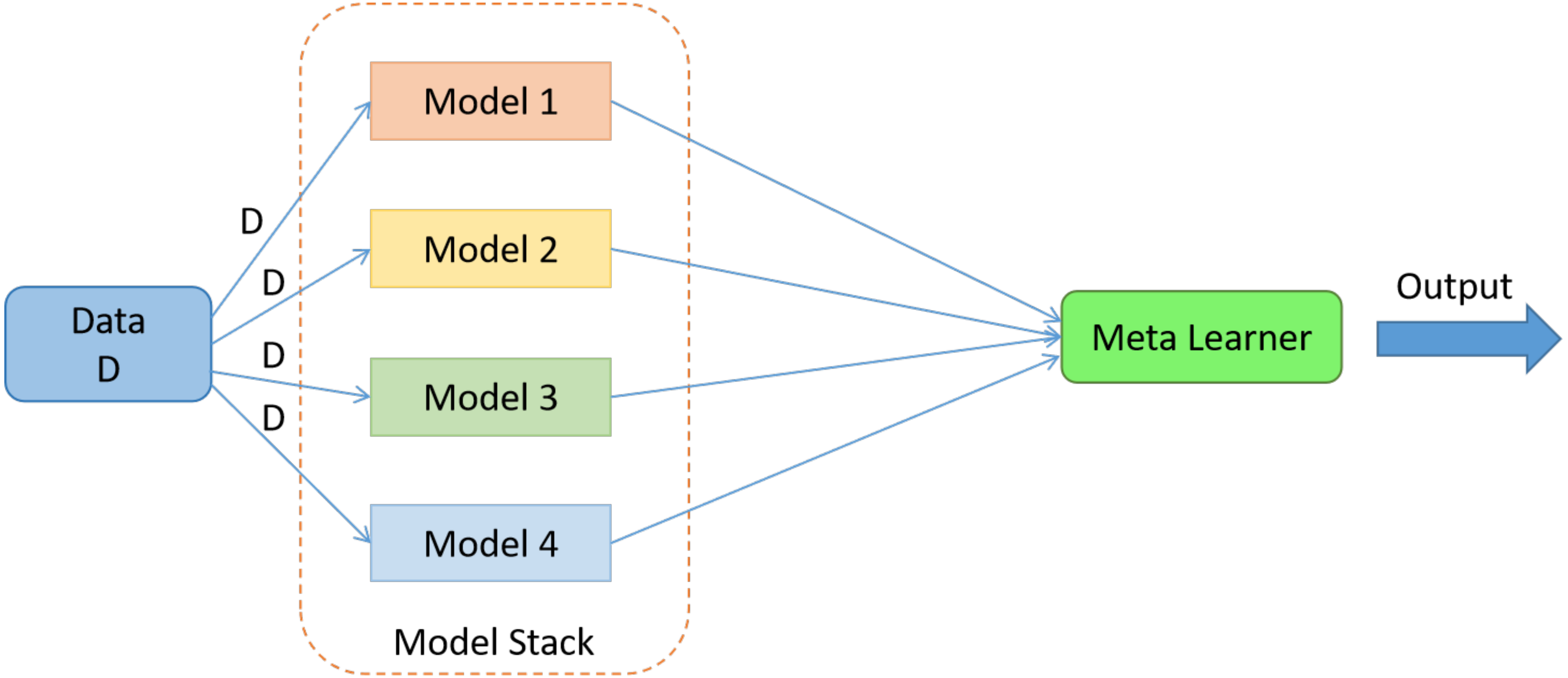


Fig. Illustration of Stacking Ensemble [52]

[52] https://www.analyticsvidhya.com/blog/2021/08/ensemble-stacking-for-machine-learning-and-deep-learning/

2.7.1. Model Ensemble

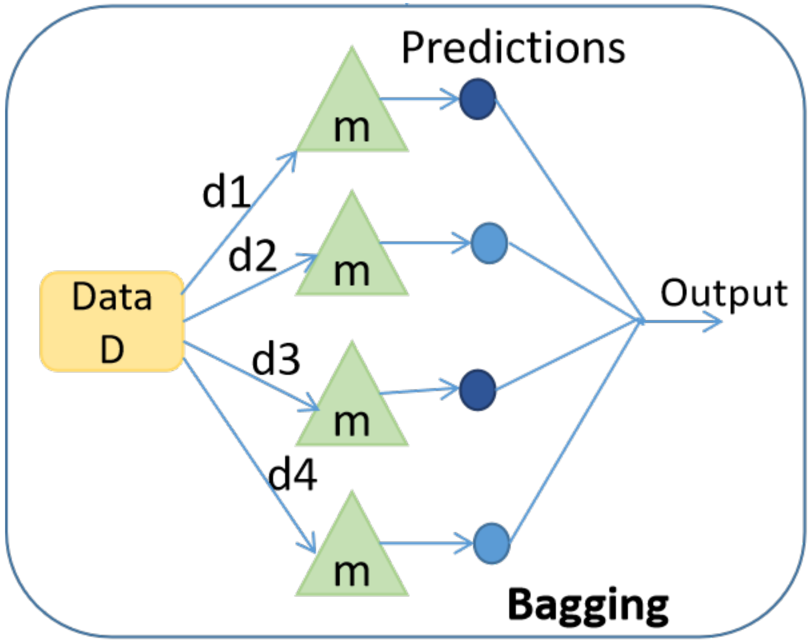


Fig. Illustration of Bagging Ensemble [52]

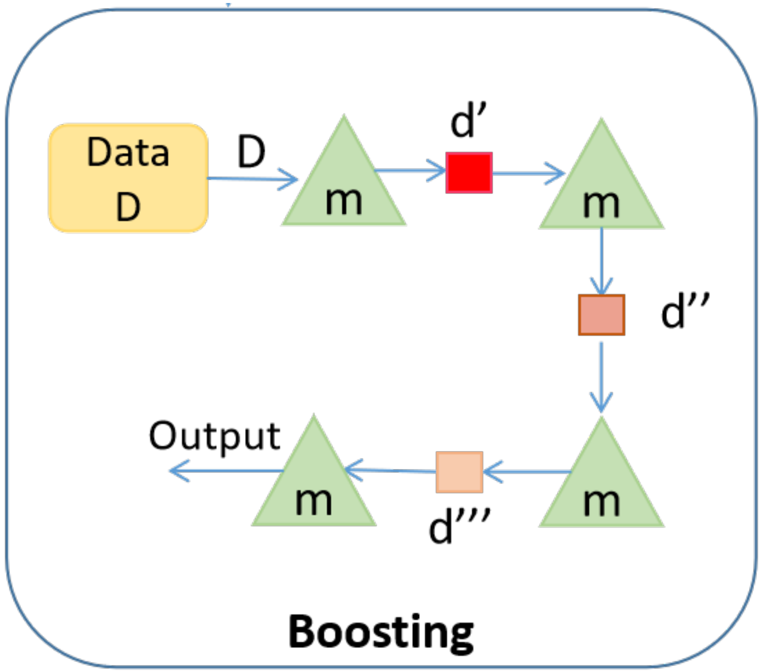


Fig. Illustration of Boosting Ensemble [52]

[52] https://www.analyticsvidhya.com/blog/2021/08/ensemble-stacking-for-machine-learning-and-deep-learning/

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.

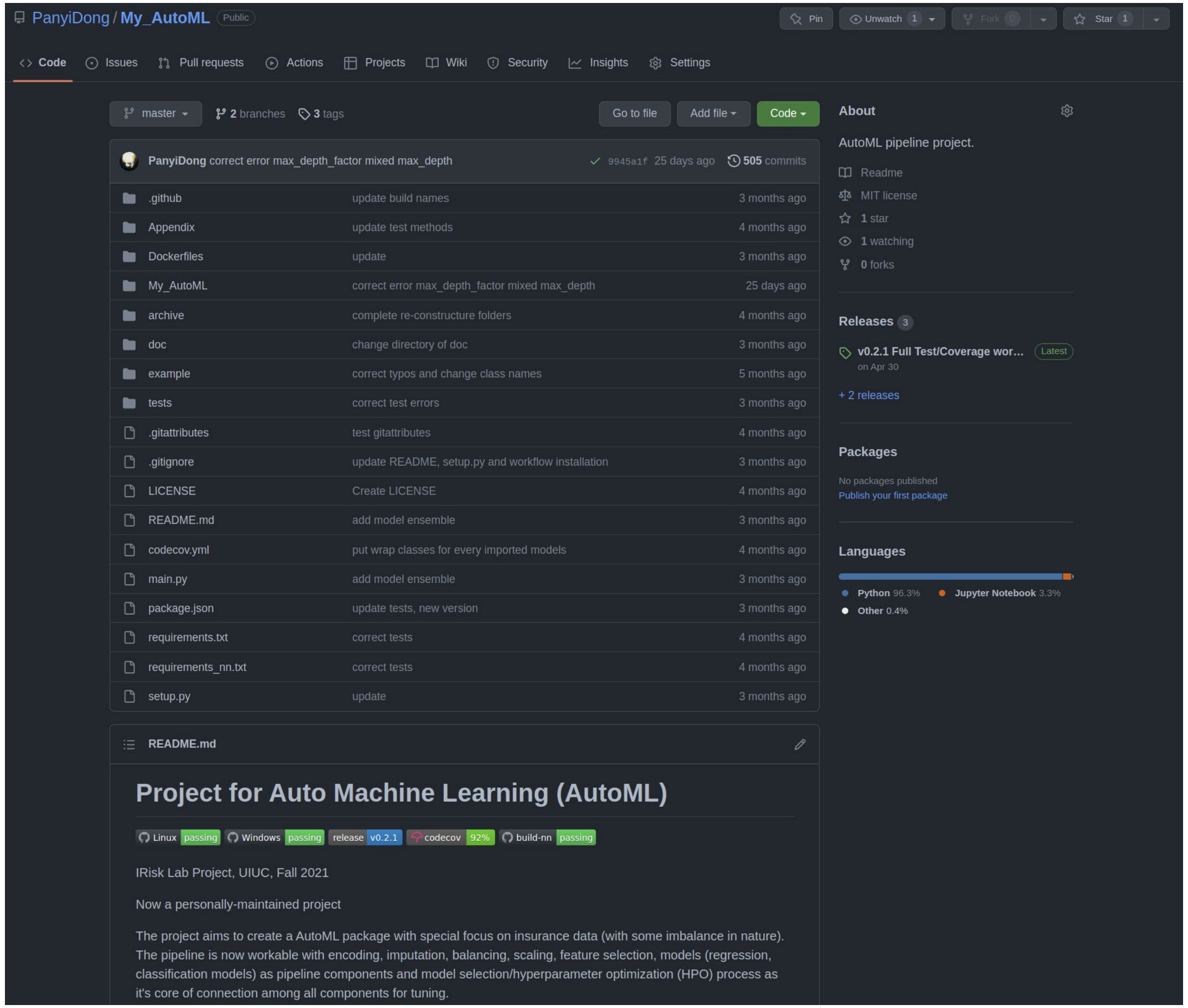
Future:

(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



PanyiDong correct error max_depth_factor mixed max_depth ✓ 9945a1f 25 days ago 505 commits

.github	update build names	3 months ago
Appendix	update test methods	4 months ago
Dockerfiles	update	3 months ago
My_AutoML	correct error max_depth_factor mixed max_depth	25 days ago
archive	complete re-constructure folders	4 months ago
doc	change directory of doc	3 months ago
example	correct typos and change class names	5 months ago
tests	correct test errors	3 months ago
.gitattributes	test gitattributes	4 months ago
.gitignore	update README, setup.py and workflow installation	3 months ago
LICENSE	Create LICENSE	4 months ago
README.md	add model ensemble	3 months ago
codecov.yml	put wrap classes for every imported models	4 months ago
main.py	add model ensemble	3 months ago
package.json	update tests, new version	3 months ago
requirements.txt	correct tests	4 months ago
requirements_nn.txt	correct tests	4 months ago
setup.py	update	3 months ago

About

AutoML pipeline project.

Readme
MIT license
1 star
1 watching
0 forks

Releases 3

v0.2.1 Full Test/Coverage wor... Latest
on Apr 30

+ 2 releases

Packages

No packages published
Publish your first package

Languages

● Python 96.3% ● Jupyter Notebook 3.3%
● Other 0.4%

README.md

Project for Auto Machine Learning (AutoML)

Linux passing | Windows passing | release v0.2.1 | codecov 92% | build-nn passing

IRisk Lab Project, UIUC, Fall 2021

Now a personally-maintained project

The project aims to create a AutoML package with special focus on insurance data (with some imbalance in nature). The pipeline is now workable with encoding, imputation, balancing, scaling, feature selection, models (regression, classification models) as pipeline components and model selection/hyperparameter optimization (HPO) process as it's core of connection among all components for tuning.

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

Thanks!

Questions