Algorithm Chains and Pipelines

ESM3081 Programming for Data Science

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Algorithm Chains and Pipelines

- Most machine learning applications require not only the application of a single algorithm, but the chaining together of many different processing steps and machine learning models.
 - *e.g.*, feature scaling, feature engineering, ...
- We will cover how to use the *Pipeline* class to simplify the process of building chains of transformations and models.
 - Combining *Pipeline* and *GridSearchCV* to search over hyperparameters for all processing steps at once.

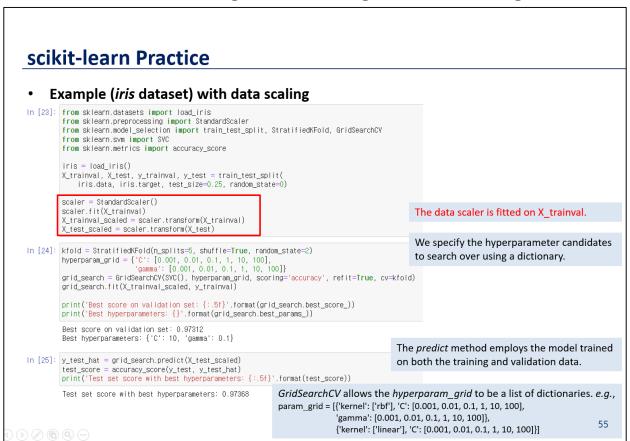
Topics

- Pipeline Interface
- Automatic Model Selection
- AutoML

Building Pipelines

Hyperparameter Selection with Preprocessing

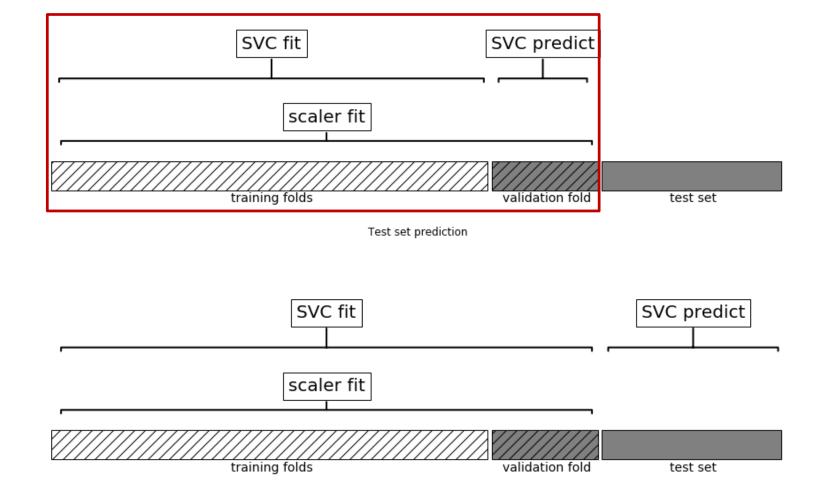
- A naïve approach to search over the hyperparameters for SVC using GridSearchCV
 - When scaling the data, we used all the data points in the training set to obtain the scaling criterion.
 - We then used the scaled training data to run grid search using cross-validation.



Hyperparameter Selection with Preprocessing

Data usage when preprocessing outside the cross-validation loop (Improper Preprocessing)

Cross validation



Pipelines

- We used the information from the entire training set, including the validation part, to find the right scaling of the data.
- This is fundamentally different from how new data looks to the model.
 - The splits in the cross-validation no longer correctly mirror how new data will look to the modeling process.
 - This will lead to overly optimistic results during cross-validation, and possibly the selection of suboptimal hyperparameters.
- To get around this problem, the splitting of the dataset during cross-validation should be done before doing any preprocessing.
 - To achieve this, we can use the Pipeline class.

https://scikit-learn.org/stable/modules/generated/sklearn.pipeline.Pipeline.html

sklearn.pipeline.Pipeline

class sklearn.pipeline.Pipeline(steps, *, memory=None, verbose=False)

[source]

Pipeline of transforms with a final estimator.

Sequentially apply a list of transforms and a final estimator. Intermediate steps of the pipeline must be 'transforms', that is, they must implement fit and transform methods. The final estimator only needs to implement fit. The transformers in the pipeline can be cached using memory argument.

The purpose of the pipeline is to assemble several steps that can be cross-validated together while setting different parameters. For this, it enables setting parameters of the various steps using their names and the parameter name separated by a '__', as in the example below. A step's estimator may be replaced entirely by setting the parameter with its name to another estimator, or a transformer removed by setting it to 'passthrough' or None.

Read more in the User Guide.

New in version 0.5.

Parameters:

steps: list

List of (name, transform) tuples (implementing fit/transform) that are chained, in the order in which they are chained, with the last object an estimator.

memory: str or object with the joblib. Memory interface, default=None

Used to cache the fitted transformers of the pipeline. By default, no caching is performed. If a string is given, it is the path to the caching directory. Enabling caching triggers a clone of the transformers before fitting. Therefore, the transformer instance given to the pipeline cannot be inspected directly. Use the attribute named_steps or steps to inspect estimators within the pipeline. Caching the transformers is advantageous when fitting is time consuming.

https://scikit-learn.org/stable/modules/generated/sklearn.pipeline.Pipeline.html

Methods

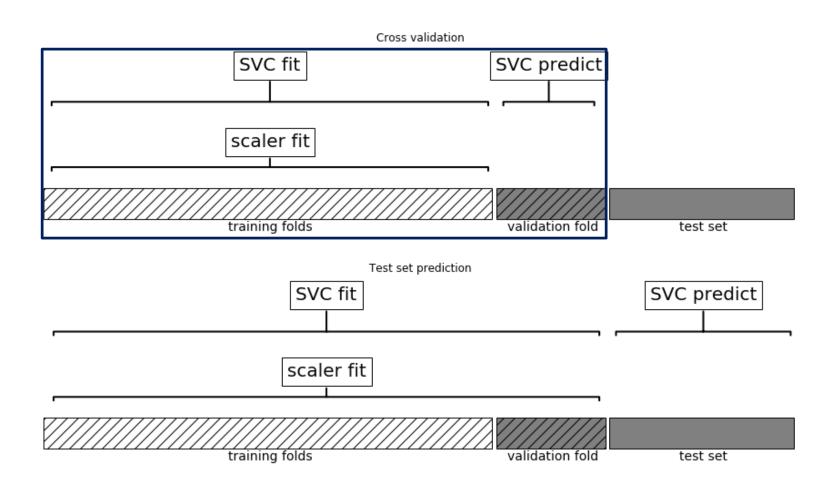
$decision_function$ (self, X)	Apply transforms, and decision_function of the final estimator
fit (self, X[, y])	Fit the model
fit_predict (self, X[, y])	Applies fit_predict of last step in pipeline after transforms.
$fit_{transform}$ (self, $X[, y]$)	Fit the model and transform with the final estimator
<pre>get_params (self[, deep])</pre>	Get parameters for this estimator.
<pre>predict (self, X, **predict_params)</pre>	Apply transforms to the data, and predict with the final estimator
predict_log_proba (self, X)	Apply transforms, and predict_log_proba of the final estimator
predict_proba (self, X)	Apply transforms, and predict_proba of the final estimator
<pre>score (self, X[, y, sample_weight])</pre>	Apply transforms, and score with the final estimator
<pre>set_params (self, **kwargs)</pre>	Set the parameters of this estimator.

Example (iris dataset) with data scaling

```
In [2]: from sklearn.datasets import load iris
        from sklearn.preprocessing import StandardScaler
        from sklearn.model_selection import train_test_split
        from sklearn.svm import SVC
        from sklearn.metrics import accuracy score
        iris = load iris()
        X trainval, X test, y trainval, y test = train test split(
            iris.data, iris.target, test_size=0.25, random_state=0)
                                                                        We use the Pipeline class to express the workflow for
                                                                        training an SVM after scaling the data with StandardScaler
In [3]: from sklearn.pipeline import Pipeline
        pipe = Pipeline([('scaler', StandardScaler()), ('svm', SVC())])
In [4]: from sklearn.model_selection import StratifiedKFold, GridSearchCV
                                                                                         Using a pipeline in a grid search works the
        kfold = StratifiedKFold(n_splits=5, shuffle=True, random_state=2)
                                                                                        same way as using any other estimator.
        hyperparam grid = \{'svm \ C': [0.001, 0.01, 0.1, 1, 10, 100],
                           'svm gamma': [0.001, 0.01, 0.1, 1, 10, 100]}
        grid_search = GridSearchCV(pipe, hyperparam_grid, scoring='accuracy', refit=True, cv=kfold)
        grid_search.fit(X_trainval, y_trainval)
        print("Best score on validation set: {:.5f}".format(grid_search.best_score_))
        print("Best hyperparameters: {}".format(grid search.best params ))
                                                                 When defining the hyperparameter grid, we need to specify for
        Best score on validation set: 0.97312
        Best hyperparameters: {'svm_C': 10, 'svm_gamma': 0.1}
                                                                 each hyperparameter which step of the pipeline it belongs to.
                                                                 Syntax: the step name, followed by (a double underscore), followed by
In [5]: y_test_hat = grid_search.predict(X_test)
                                                                 the hyperparameter name
        test_score = accuracy_score(y_test, y_test_hat)
        print("Test set score with best hyperparameters: {:.5f}".format(test score))
                                                                                                                                    10
        Test set score with best hyperparameters: 0.97368
```

Discussion

Data usage when preprocessing inside the cross-validation loop with a pipeline



Discussion

- Using the pipeline, we can encapsulate all the processing steps in the machine learning workflow in a single estimator.
- We can reduce the code needed for our "preprocessing + classification" process.
- In contrast to the grid search we did before, now for each split in the crossvalidation, the scaler is refit with only the training part.

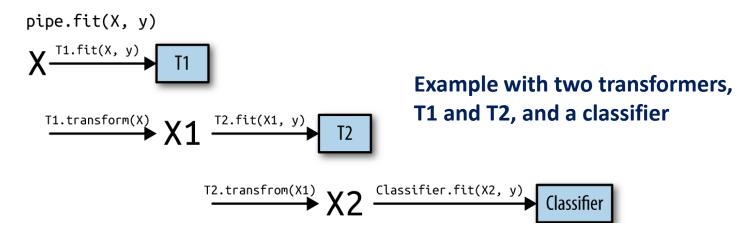
General Pipeline Interface

Pipeline Interface

- The Pipeline class is not restricted to preprocessing and classification, but can in fact join any number of estimators together.
 - For example, you could build a pipeline containing feature engineering, feature selection, feature scaling, and classification, for a total of four steps.
 - The last step could be regression or clustering instead of classification.
- The only requirement for estimators in a pipeline is
 - All but the last step need to have a transform method, so they can produce a new representation of the data that can be used in the next step.
 - The last step of a pipeline is only required to have a fit method.

Pipeline Interface

- Overview of the pipeline training and prediction process
 - **Training process**: the pipeline calls fit and then transform on each step in turn, with the input given by the output of the transform method of the previous step. For the last step in the pipeline, just fit is called.



- **Prediction process:** the pipeline transforms the data using all but the last step, and then predicts on the last step.

pipe.predict(X')
$$X \xrightarrow{\text{T1.transform}(X')} X \xrightarrow{\text{1}} 1 \xrightarrow{\text{T2.transform}(X'1)} X \xrightarrow{\text{2}} 2 \xrightarrow{\text{Classifier.predict}(X'2)} y$$

Pipeline Creation

- There is a convenience function make_pipeline that will create a pipeline for us and automatically name each step based on its class.
 - Example syntax for make_pipeline

```
from sklearn.pipeline import make_pipeline
# standard syntax
pipe_long = Pipeline([("scaler", MinMaxScaler()), ("svm", SVC(C=100))])
# abbreviated syntax
pipe short = make pipeline(MinMaxScaler(), SVC(C=100))
print("Pipeline steps:\n{}".format(pipe_short.steps))
   Pipeline steps:
   [('minmaxscaler', MinMaxScaler(copy=True, feature range=(0, 1))),
    ('svc', SVC(C=100, cache_size=200, class_weight=None, coef0=0.0,
                decision function shape='ovr', degree=3, gamma='auto',
                kernel='rbf', max iter=-1, probability=False,
                random_state=None, shrinking=True, tol=0.001,
                verbose=False))]
```

Accessing Attributes in a Pipeline

- You can inspect attributes of one of the steps of the pipeline.
 - *pipeline.steps* is a list of tuples, so *pipeline.steps*[0][1] is the first estimator, *pipeline.steps*[1][1] is the second estimator, and so on.
 - The easiest way to access each step in a pipeline is via the *named_steps* attribute, which is a dictionary from the step names to the estimators.
 - Example syntax for named_step attribute

```
from sklearn.preprocessing import StandardScaler
from sklearn.decomposition import PCA
pipe = make pipeline(StandardScaler(), PCA(n components=2), StandardScaler())
print("Pipeline steps:\n{}".format(pipe.steps))
   Pipeline steps:
   [('standardscaler-1', StandardScaler(copy=True, with_mean=True, with_std=True)),
    ('pca', PCA(copy=True, iterated_power='auto', n_components=2, random_state=None,
               svd_solver='auto', tol=0.0, whiten=False)),
    ('standardscaler-2', StandardScaler(copy=True, with mean=True, with std=True))]
# fit the pipeline defined before to the cancer dataset
pipe.fit(cancer.data)
# extract the first two principal components from the "pca" step
components = pipe.named steps["pca"].components
print("components.shape: {}".format(components.shape))
   components.shape: (2, 30)
```

Automatic Model Selection

Grid-Searching Which Model To Use

- One of the main reasons to use Pipeline is for doing grid searches.
- Combining GridSearchCV and Pipeline makes is possible to search over the actual steps being performed in the pipeline.
 - This leads to an even bigger search space.
 - Trying all possible solutions is usually not a viable machine learning strategy, thus it should be considered carefully.
 - Example: Comparing an SVC, an MLPClassifier and a RandomForestClassifier
 - The SVC might need the data to be scaled, so we also search over whether to use StandardScaler, MinMaxScaler or None(no preprocessing).
 - The MLPClassifier might also need the data to be scaled.
 - For the RandomForestClassifier, we know that no preprocessing is necessary.
 - Because they have different hyperparameters to tune, and need different preprocessing, we can make use of the list of search grids

Example (breast_cancer dataset)

```
In [6]: from sklearn.datasets import load_breast_cancer
        from sklearn.model selection import train test split
        from sklearn.pipeline import Pipeline
        from sklearn, preprocessing import StandardScaler, MinMaxScaler
        from sklearn.svm import SVC
        from sklearn.neural_network import MLPClassifier
        from sklearn.ensemble import RandomForestClassifier
                                                                                       We start by defining the pipeline. We can
        from sklearn.model selection import StratifiedKFold, GridSearchCV
                                                                                       instantiate this pipeline using any estimators.
        cancer = load breast cancer()
        X_train, X_test, y_train, y_test = train_test_split(cancer.data, cancer.target, random_state=0)
In [7]: pipe = Pipeline([('preprocessing', None), ('classifier', SVC())])
        hyperparam grid = [
            {'classifier': [SVC()], 'preprocessing': [StandardScaler(), MinMaxScaler(), None],
             'classifier__gamma': [0.001, 0.01, 0.1, 1, 10, 100],
             'classifier__C': [0.001, 0.01, 0.1, 1, 10, 100]},
            {'classifier': [MLPClassifier(solver='lbfgs')], 'preprocessing': [StandardScaler(), MinMaxScaler(), None],
             'classifier_hidden_layer_sizes': [(10,), (20,), (50,), (100,)],
             'classifier activation': ['tanh', 'relu']},
                                                                                                  We make use of the list of search
            {'classifier': [RandomForestClassifier(n_estimators=100)],
                                                                                                  grids.
             'preprocessing': [None], 'classifier max features': [1, 2, 3]}]
        kfold = StratifiedKFold(n_splits=5, shuffle=True, random_state=1)
        grid = GridSearchCY(pipe, hyperparam_grid, scoring='accuracy', refit=True, cv=kfold)
        grid.fit(X train, y train)
                                                                                           Now we instantiate and run the grid
        print("Best hyperparams:\foothat(grid.best_params_))
                                                                                           search as usual.
        print("Best cross-validation score: {:.5f}".format(grid.best score ))
        print("Test-set score: {:.5f}".format(grid.score(X_test, y_test)))
```

Example (breast_cancer dataset)

- Example (breast_cancer dataset)
 - Accessing Attributes in a Pipeline



The best model found by GridSearchCV is stored in *grid.best_estimator_*.

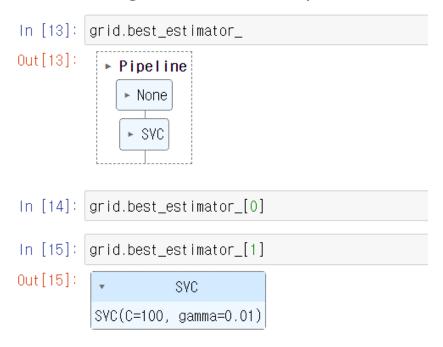
We can access each step in a pipeline via the *named_steps* attribute.

Example (iris dataset)

```
In [11]: from sklearn.datasets import load iris
         from sklearn.model_selection import train_test_split
         from sklearn.pipeline import Pipeline
         from sklearn.preprocessing import StandardScaler, MinMaxScaler
         from sklearn.svm import SVC
         from sklearn.neural network import MLPClassifier
         from sklearn.ensemble import RandomForestClassifier
                                                                                           We start by defining the pipeline. We can
         from sklearn.model_selection import StratifiedKFold, GridSearchCV
                                                                                           instantiate this pipeline using any estimators.
         iris = load iris()
         X_train, X_test, y_train, y_test = train_test_split(iris.data, iris.target, random_state=0)
In [12]: pipe = Pipeline([('preprocessing', None), ('classifier', SVC())])
         hyperparam grid = [
             {'classifier': [SYC()], 'preprocessing': [StandardScaler(), MinMaxScaler(), None],
              'classifier__gamma': [0.001, 0.01, 0.1, 1, 10, 100],
              'classifier__C': [0.001, 0.01, 0.1, 1, 10, 100]},
             {'classifier': [MLPClassifier(solver='lbfgs')], 'preprocessing': [StandardScaler(), MinMaxScaler(), None],
              'classifier_hidden_layer_sizes': [(10,), (20,), (50,), (100,)],
              'classifier__activation': ['tanh', 'relu']},
                                                                                                      We make use of the list of search
             {'classifier': [RandomForestClassifier(n_estimators=100)],
                                                                                                      grids.
              'preprocessing': [None], 'classifier__max_features': [1, 2, 3]}]
         kfold = StratifiedKFold(n_splits=5, shuffle=True, random_state=1)
         grid = GridSearchCV(pipe, hyperparam_grid, scoring='accuracy', refit=True, cv=kfold)
         grid.fit(X_train, y_train)
                                                                                               Now we instantiate and run the grid
         print('Best estimator:\(\psi_\)'.format(grid.best_estimator_))
         print('Best hyperparams:\footnote{\text{nf}}'.format(grid.best params ))
                                                                                               search as usual.
         print('Best cross-validation score: {:.5f}'.format(grid.best_score_))
         print('Test-set score: {:.5f}'.format(grid.score(X test, y test)))
```

Example (iris dataset)

- Example (iris dataset)
 - Accessing Attributes in a Pipeline



The best model found by GridSearchCV is stored in grid.best_estimator_

We can also access each step in a pipeline using index

Discussion

- We can search over the data preprocessing strategies using the outcome of a supervised task like regression or classification.
- Searching over preprocessing hyperparameters together with model hyper parameters is a very powerful strategy.
 - Keep in mind that GridSearchCV tries *all possible combinations* of the specified hyperparameters.
 - Adding more hyperparameters to the grid exponentially increases the number of models that need to be built.

Summary and Outlook

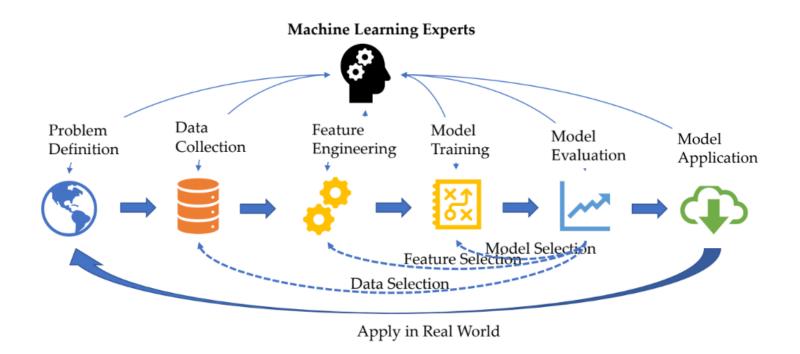
Summary and Outlook

- The Pipeline class is a general-purpose tool to chain together multiple processing steps in a machine learning workflow.
- Using pipelines allows us to encapsulate multiple steps into a single Python object that adheres to the familiar scikit-learn interface of fit, predict, and transform.
 - Real-world applications of machine learning involves a sequence of processing steps.
 - Choosing the right combination of feature engineering, preprocessing, and models is somewhat of an art, and often requires some trial and error.
 - Using pipelines, this "trying out" of many different processing steps is quite simple.
 - Also, the Pipeline class allows writing more succinct code.
- We now possess all the required skills and know the necessary mechanisms to apply machine learning in practice.

Automated Machine Learning

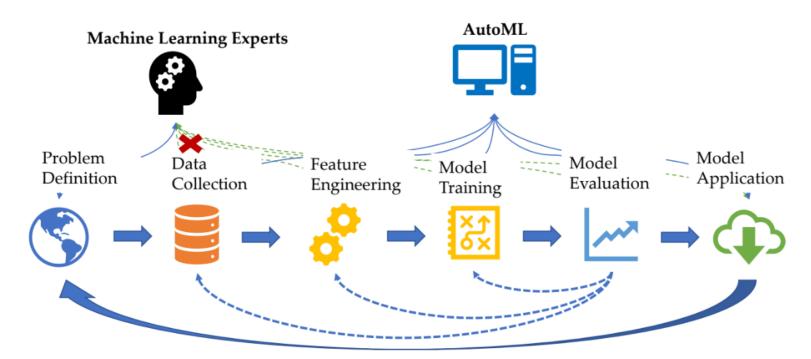
AutoML

 The success of machine learning (ML) in real-world applications crucially relies on human ML experts to perform the following tasks

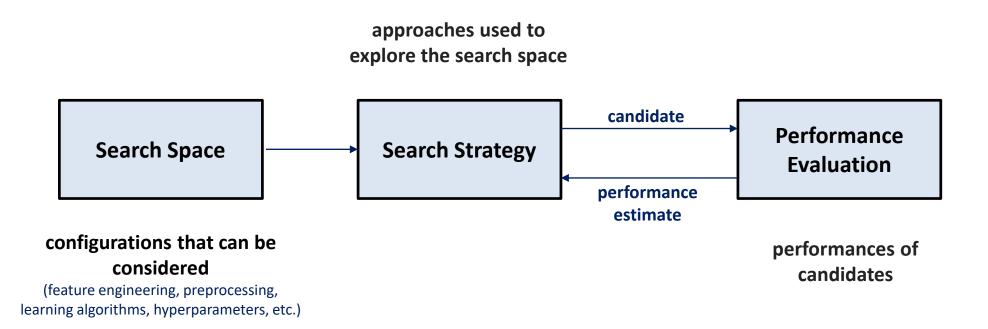


AutoML

- As the complexity of these tasks is often beyond non-ML-experts, the rapid growth of machine learning applications has created a demand for off-the-shelf machine learning methods that can be used easily and without expert knowledge.
- Automated Machine Learning (AutoML) is the process of automating end-to-end the process of applying machine learning to real-world problems.



AutoML



Feurer, M., Klein, A., Eggensperger, K., Springenberg, J., Blum, M., & Hutter, F. (2015). Efficient and robust automated machine learning. In *Advances in Neural Information Processing Systems* (pp. 2962-2970).

Efficient and Robust Automated Machine Learning

Matthias Feurer Jost Tobias Springenberg Aaron Klein Manuel Blum Katharina Eggensperger Frank Hutter

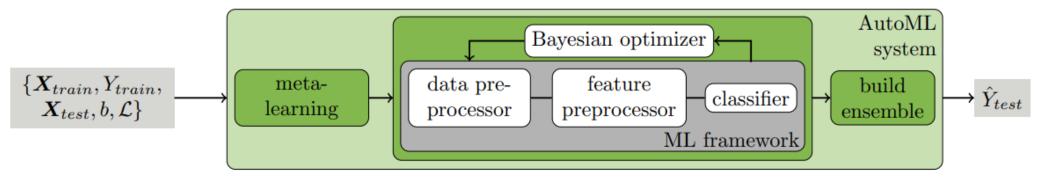
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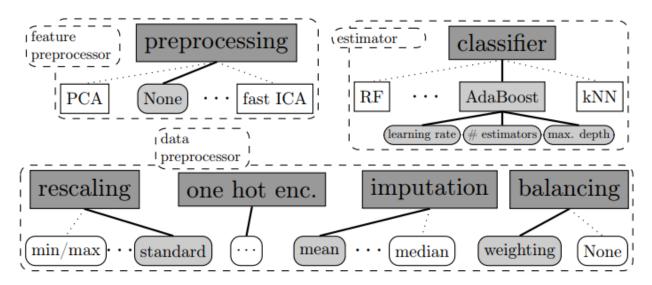
Abstract

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.

Pipeline



Search Space



https://automl.github.io/auto-sklearn/

auto-sklearn

auto-sklearn is an automated machine learning toolkit and a drop-in replacement for a scikit-learn estimator:

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

auto-sklearn frees a machine learning user from algorithm selection and hyperparameter tuning. It leverages recent advantages in *Bayesian optimization*, *meta-learning* and *ensemble construction*. Learn more about the technology behind *auto-sklearn* by reading our paper published at NIPS 2015.

NEW: Auto-sklearn 2.0

Auto-sklearn 2.0 includes latest research on automatically configuring the AutoML system itself and contains a multitude of improvements which speed up the fitting the AutoML system.

auto-sklearn 2.0 works the same way as regular auto-sklearn and you can use it via

```
>>> from autosklearn.experimental.askl2 import AutoSklearn2Classifier
```

https://automl.github.io/auto-sklearn/

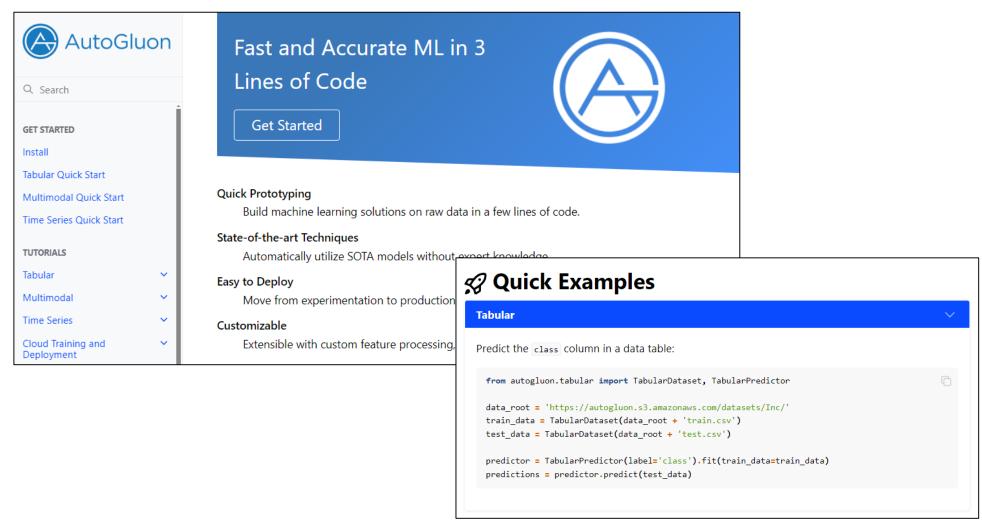
Example

```
>>> import autosklearn.classification
>>> import sklearn.model selection
>>> import sklearn.datasets
>>> import sklearn.metrics
>>> if name == " main ":
       X, y = sklearn.datasets.load_digits(return_X_y=True)
>>>
       X train, X test, y train, y test = \
>>>
           sklearn.model selection.train test split(X, y, random_state=1)
        automl = autosklearn.classification.AutoSklearnClassifier()
>>>
       automl.fit(X train, y train)
>>>
       y_hat = automl.predict(X test)
>>>
       print("Accuracy score", sklearn.metrics.accuracy score(y test, y hat))
>>>
```

This will run for one hour and should result in an accuracy above 0.98.

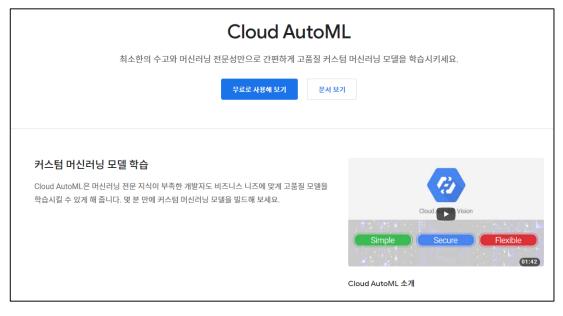
AutoGluon

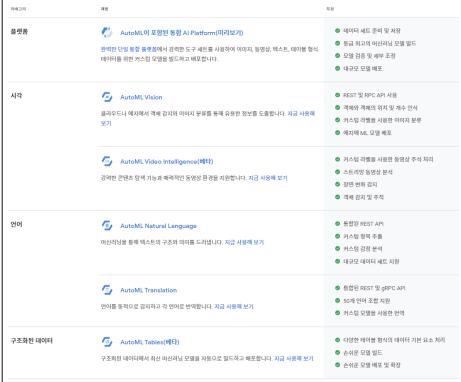
https://auto.gluon.ai/



Google Cloud AutoML

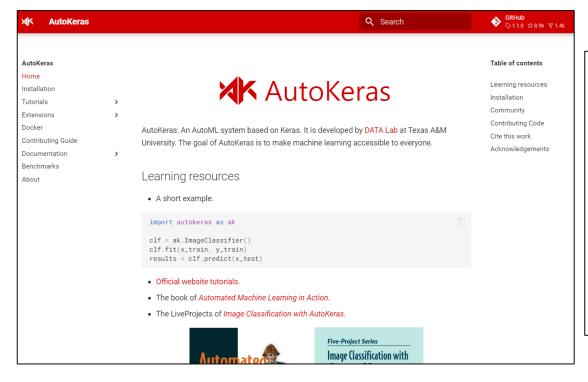
https://cloud.google.com/automl





AutoKeras

https://autokeras.com/



Supported Tasks

AutoKeras supports several tasks with an extremely simple interface. You can click the links below to see the detailed tutorial for each task.

Supported Tasks:

Image Classification

Image Regression

Text Classification

Text Regression

Structured Data Classification

Structured Data Regression

Coming Soon: Time Series Forecasting, Object Detection, Image Segmentation.

H2O Driverless Al

https://h2o.ai/platform/ai-cloud/make/h2o-driverless-ai/



