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.

scikit-learn Practice

- **Example (*iris* dataset) with data scaling**

```
In [23]: from sklearn.datasets import load_iris
         from sklearn.preprocessing import StandardScaler
         from sklearn.model_selection import train_test_split, StratifiedKFold, GridSearchCV
         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)

         scaler = StandardScaler()
         scaler.fit(X_trainval)
         X_trainval_scaled = scaler.transform(X_trainval)
         X_test_scaled = scaler.transform(X_test)
```

The data scaler is fitted on X_trainval.

```
In [24]: kfold = StratifiedKFold(n_splits=5, shuffle=True, random_state=2)
         hyperparam_grid = {'C': [0.001, 0.01, 0.1, 1, 10, 100],
                            'gamma': [0.001, 0.01, 0.1, 1, 10, 100]}
         grid_search = GridSearchCV(SVC(), hyperparam_grid, scoring='accuracy', refit=True, cv=kfold)
         grid_search.fit(X_trainval_scaled, y_trainval)

         print('Best score on validation set: {:.5f}'.format(grid_search.best_score_))
         print('Best hyperparameters: {}'.format(grid_search.best_params_))

         Best score on validation set: 0.97312
         Best hyperparameters: {'C': 10, 'gamma': 0.1}
```

We specify the hyperparameter candidates to search over using a dictionary.

```
In [25]: y_test_hat = grid_search.predict(X_test_scaled)
         test_score = accuracy_score(y_test, y_test_hat)
         print('Test set score with best hyperparameters: {:.5f}'.format(test_score))

         Test set score with best hyperparameters: 0.97368
```

The *predict* method employs the model trained on both the training and validation data.

GridSearchCV allows the *hyperparam_grid* to be a list of dictionaries. *e.g.*,

```
param_grid = [{'kernel': ['rbf'], 'C': [0.001, 0.01, 0.1, 1, 10, 100],
               'gamma': [0.001, 0.01, 0.1, 1, 10, 100]},
              {'kernel': ['linear'], 'C': [0.001, 0.01, 0.1, 1, 10, 100]}]
```

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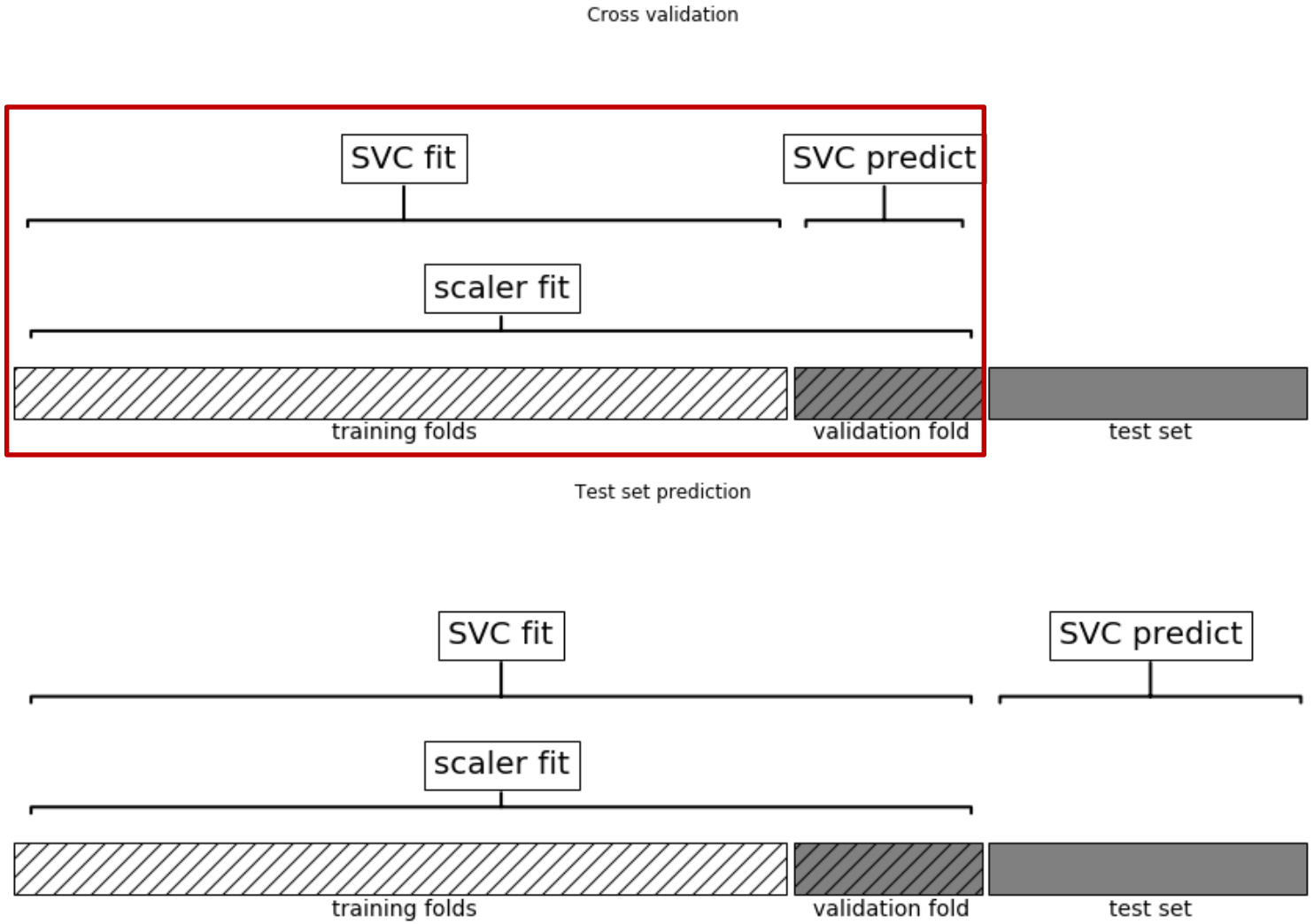
Hyperparameter Selection with Preprocessing

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



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.

scikit-learn Practice

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.

scikit-learn Practice

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
`get_params` (self[, deep])	Get parameters for this estimator.
`predict` (self, X, **predict_params)	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
`score` (self, X[, y, sample_weight])	Apply transforms, and score with the final estimator
`set_params` (self, **kwargs)	Set the parameters of this estimator.

scikit-learn Practice

- **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

kfold = StratifiedKFold(n_splits=5, shuffle=True, random_state=2)
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_))
```

```
Best score on validation set: 0.97312
Best hyperparameters: {'svm__C': 10, 'svm__gamma': 0.1}
```

Using a pipeline in a grid search works the same way as using any other estimator.

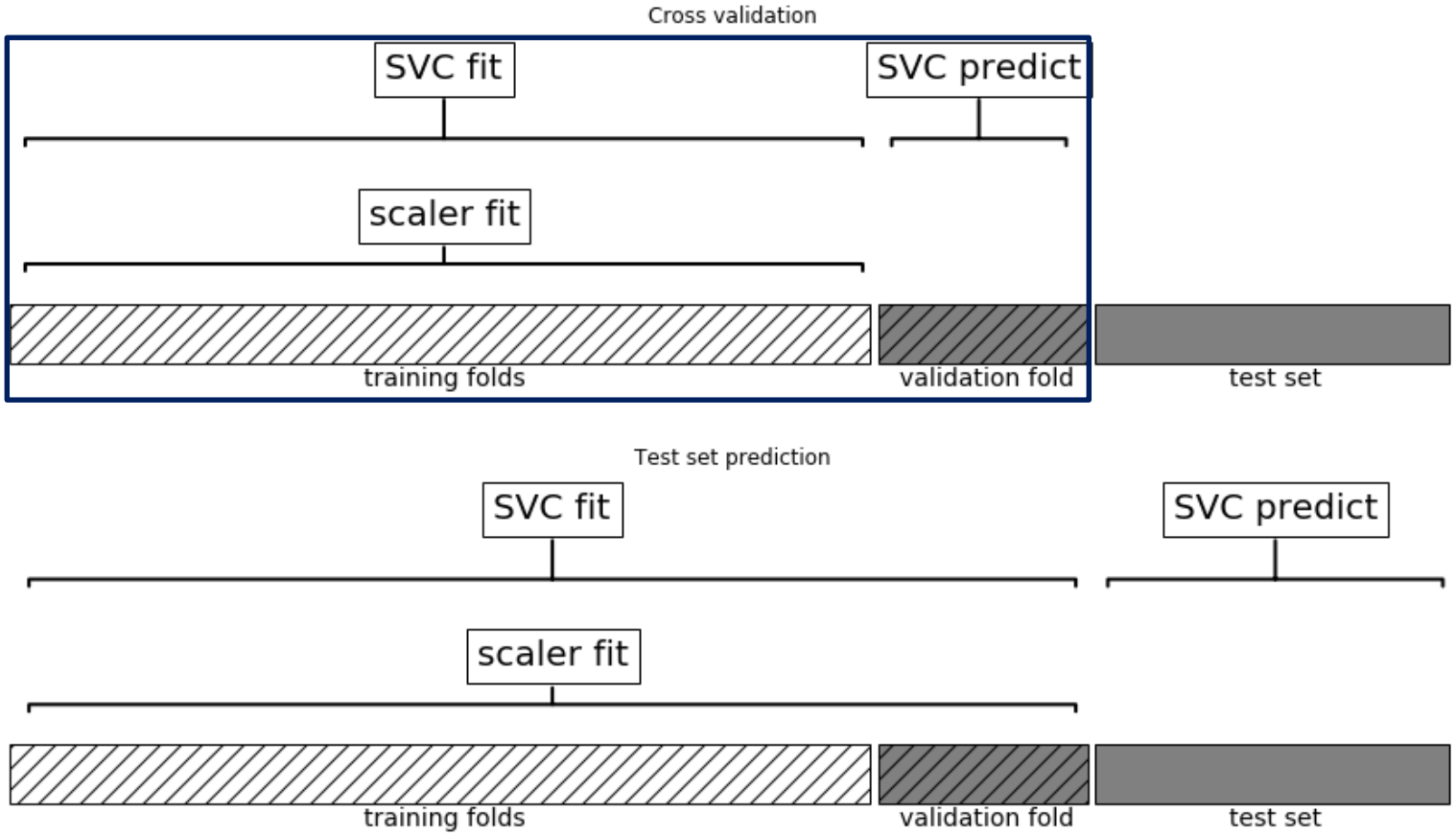
When defining the hyperparameter grid, we need to specify for each hyperparameter which step of the pipeline it belongs to.
Syntax: the step name, followed by __ (a double underscore), followed by the hyperparameter name

In [5]:
```
y_test_hat = grid_search.predict(X_test)
test_score = accuracy_score(y_test, y_test_hat)
print("Test set score with best hyperparameters: {:.5f}".format(test_score))
```

```
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 cross-validation, the scaler is refit with only the training part.**

General Pipeline Interface

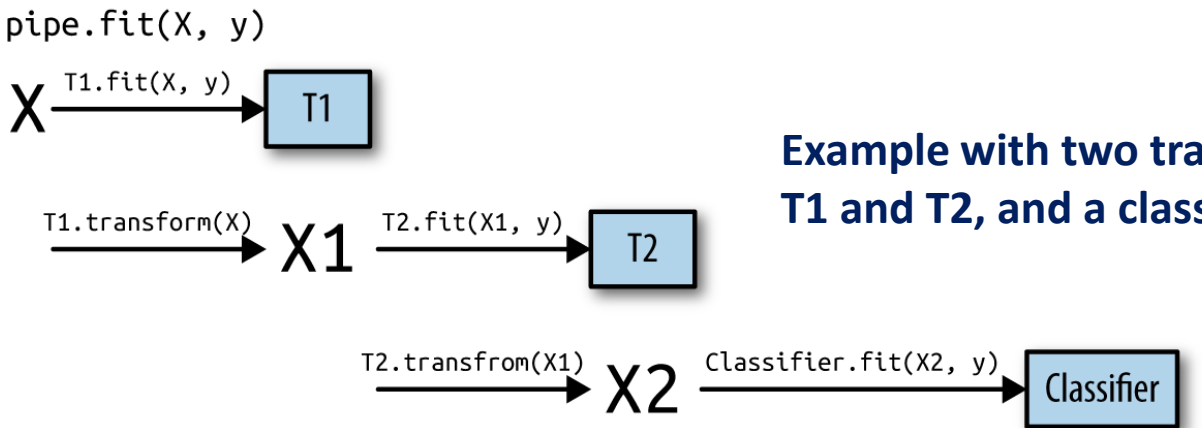
Pipeline Interface

- 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.

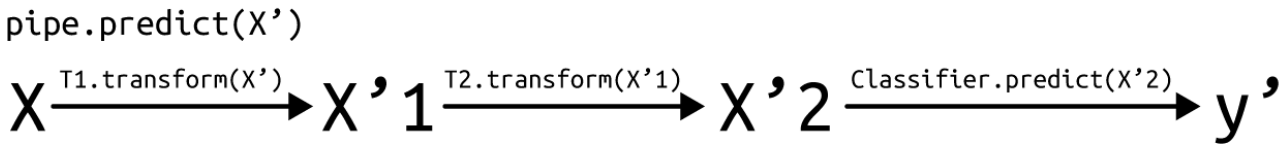
Pipeline Interface

- 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.



Example with two transformers, T1 and T2, and a classifier

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



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

scikit-learn Practice

- **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
from sklearn.model_selection import StratifiedKFold, GridSearchCV

cancer = load_breast_cancer()
X_train, X_test, y_train, y_test = train_test_split(cancer.data, cancer.target, random_state=0)
```

We start by defining the pipeline. We can instantiate this pipeline using any estimators.

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']},
    {'classifier': [RandomForestClassifier(n_estimators=100)],
     '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)

print("Best hyperparams:₩n{}".format(grid.best_params_))
print("Best cross-validation score: {:.5f}".format(grid.best_score_))
print("Test-set score: {:.5f}".format(grid.score(X_test, y_test)))
```

We make use of the list of search grids.

Now we instantiate and run the grid search as usual.

scikit-learn Practice

- **Example (*breast_cancer* dataset)**

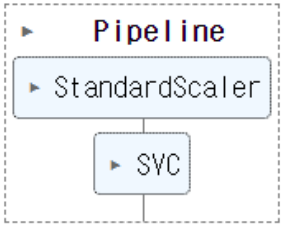
```
Best hyperparams: {
        'classifier': SVC(C=10, gamma=0.01),
                        'classifier__C': 10,
                        'classifier__gamma': 0.01,
        'preprocessing': StandardScaler()
}

Best cross-validation score: 0.97882
Test-set score: 0.97902
```

scikit-learn Practice

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

```
In [8]: grid.best_estimator_
```

Out[8]:




```
In [9]: grid.best_estimator_.named_steps['preprocessing']
```

Out[9]:

```
StandardScaler()
```

```
In [10]: grid.best_estimator_.named_steps['classifier']
```

Out[10]:

```
SVC(C=10, gamma=0.01)
```

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.

scikit-learn Practice

- **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
from sklearn.model_selection import StratifiedKFold, GridSearchCV

iris = load_iris()
X_train, X_test, y_train, y_test = train_test_split(iris.data, iris.target, random_state=0)
```

We start by defining the pipeline. We can instantiate this pipeline using any estimators.

In [12]:
```
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']},
    {'classifier': [RandomForestClassifier(n_estimators=100)],
     '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)

print('Best estimator:₩n{}'.format(grid.best_estimator_))
print('Best hyperparams:₩n{}'.format(grid.best_params_))
print('Best cross-validation score: {:.5f}'.format(grid.best_score_))
print('Test-set score: {:.5f}'.format(grid.score(X_test, y_test)))
```

We make use of the list of search grids.

Now we instantiate and run the grid search as usual.

scikit-learn Practice

- **Example (*iris* dataset)**

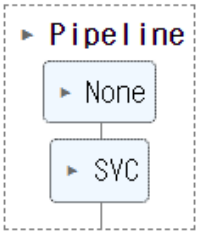
```
Best hyperparams:{
        'classifier': SVC(C=100, gamma=0.01),
                        'classifier__C': 100,
                        'classifier__gamma': 0.01,
        'preprocessing': None
}

Best cross-validation score: 0.98221
Test-set score: 0.97368
```

scikit-learn Practice

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

```
In [13]: grid.best_estimator_
```

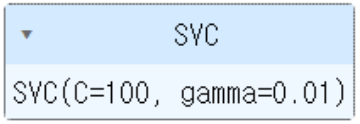
Out[13]:




```
In [14]: grid.best_estimator_[0]
```

```
In [15]: grid.best_estimator_[1]
```

Out[15]:



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.**

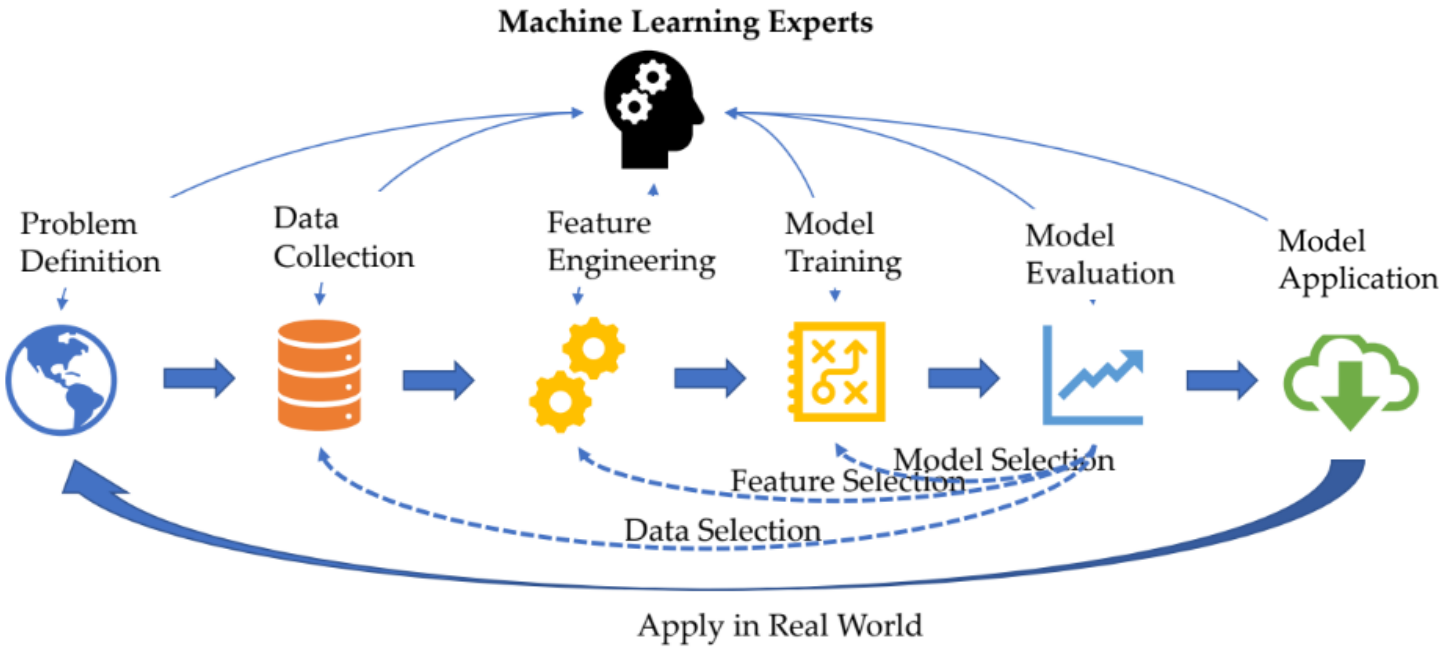
- **Using pipelines allows us to encapsulate multiple steps into a single Python object that adheres to the familiar scikit-learn interface of fit, predict, and transform.**
  - Real-world applications of machine learning involves a sequence of processing steps.
  - Choosing the right combination of 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

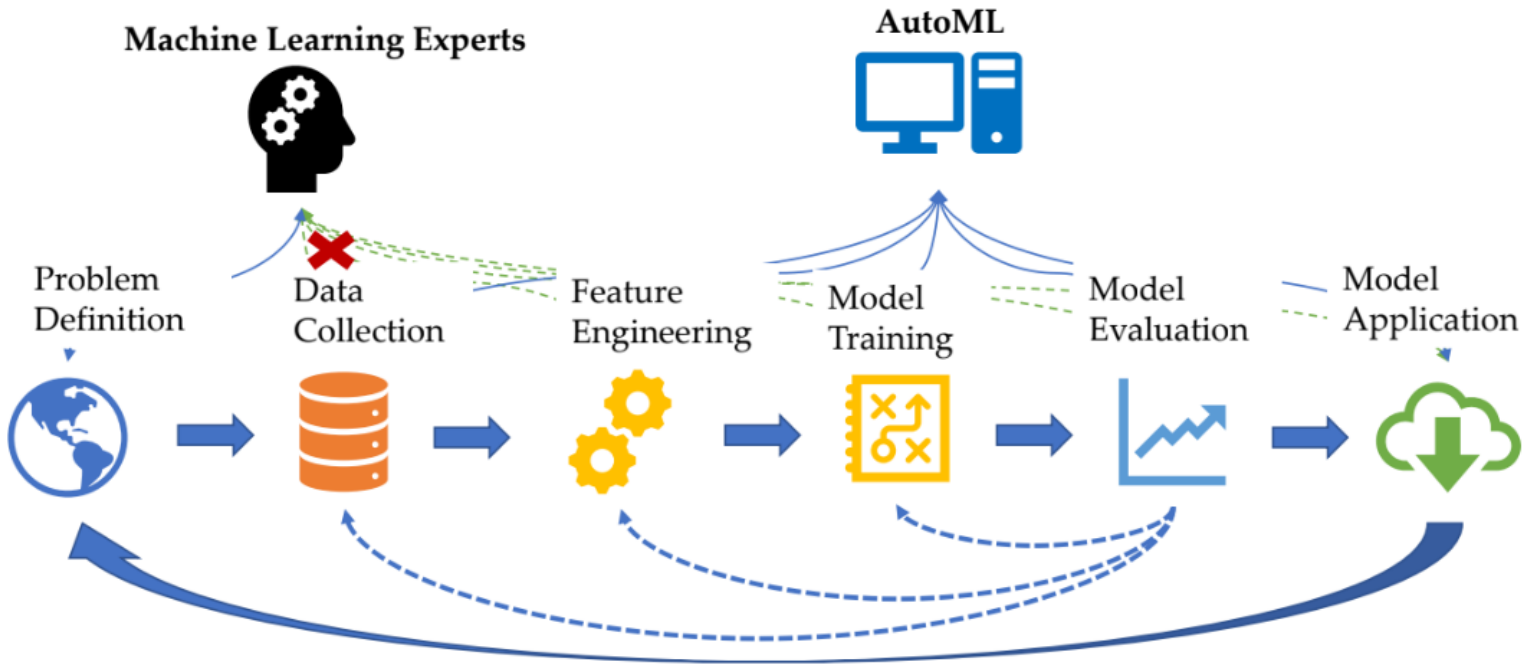
AutoML

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

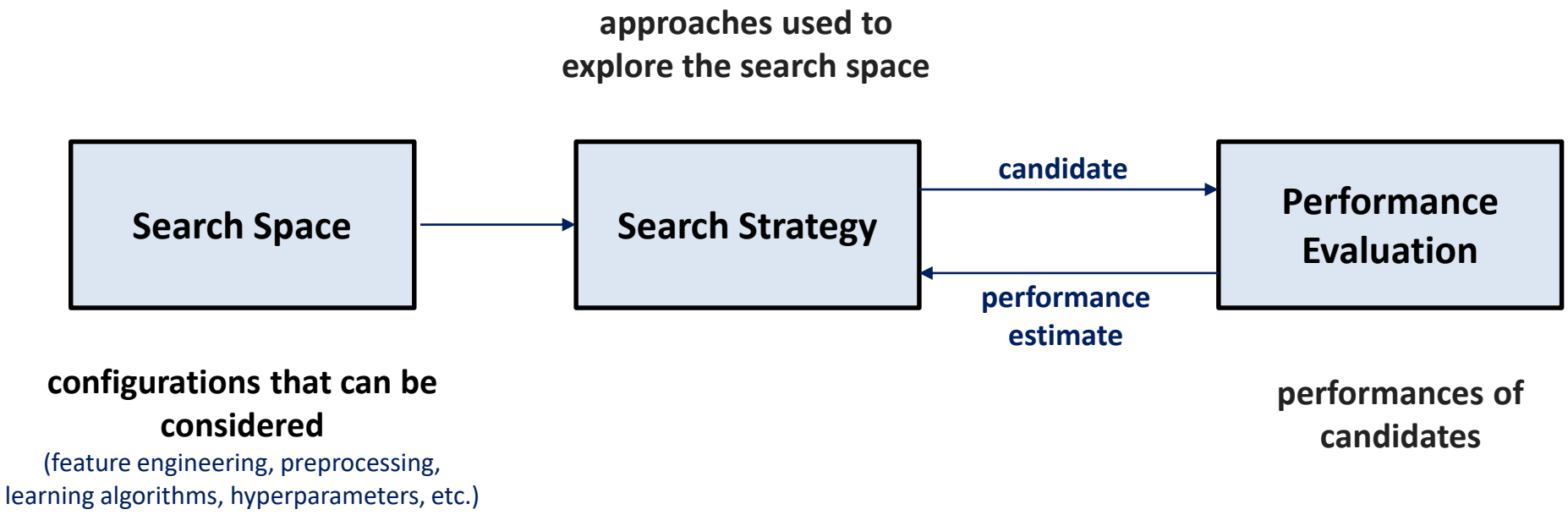


AutoML

- **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


approaches used to
explore the search space
Search Space
Search Strategy
candidate
Performance
Evaluation
performance
estimate
configurations that can be
considered
(feature engineering, preprocessing,
learning algorithms, hyperparameters, etc.)
performances of
candidates

auto-sklearn

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

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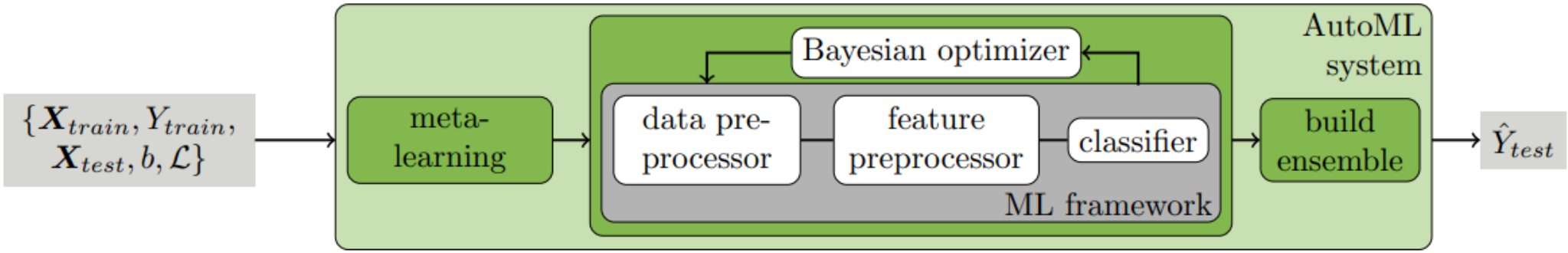
Abstract

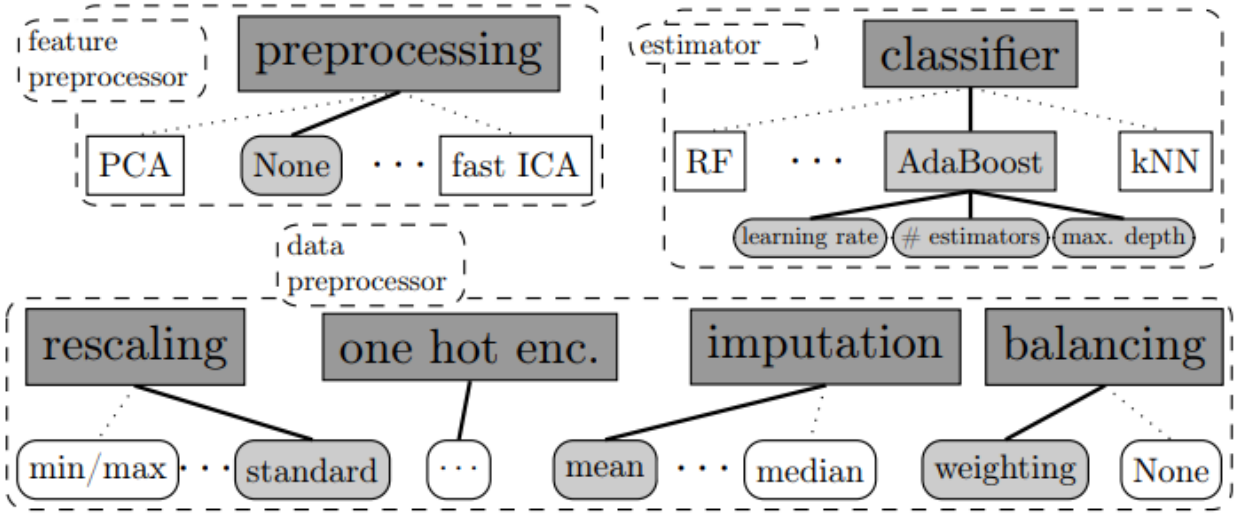
The success of machine learning in a broad range of applications has led to an ever-growing demand for machine learning systems that can be used off the shelf by non-experts. To be effective in practice, such systems need to automatically choose a good algorithm and feature preprocessing steps for a 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.

auto-sklearn

- **Pipeline**



- **Search Space**



auto-sklearn

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
```

A paper describing our advances is available on arXiv.

auto-sklearn

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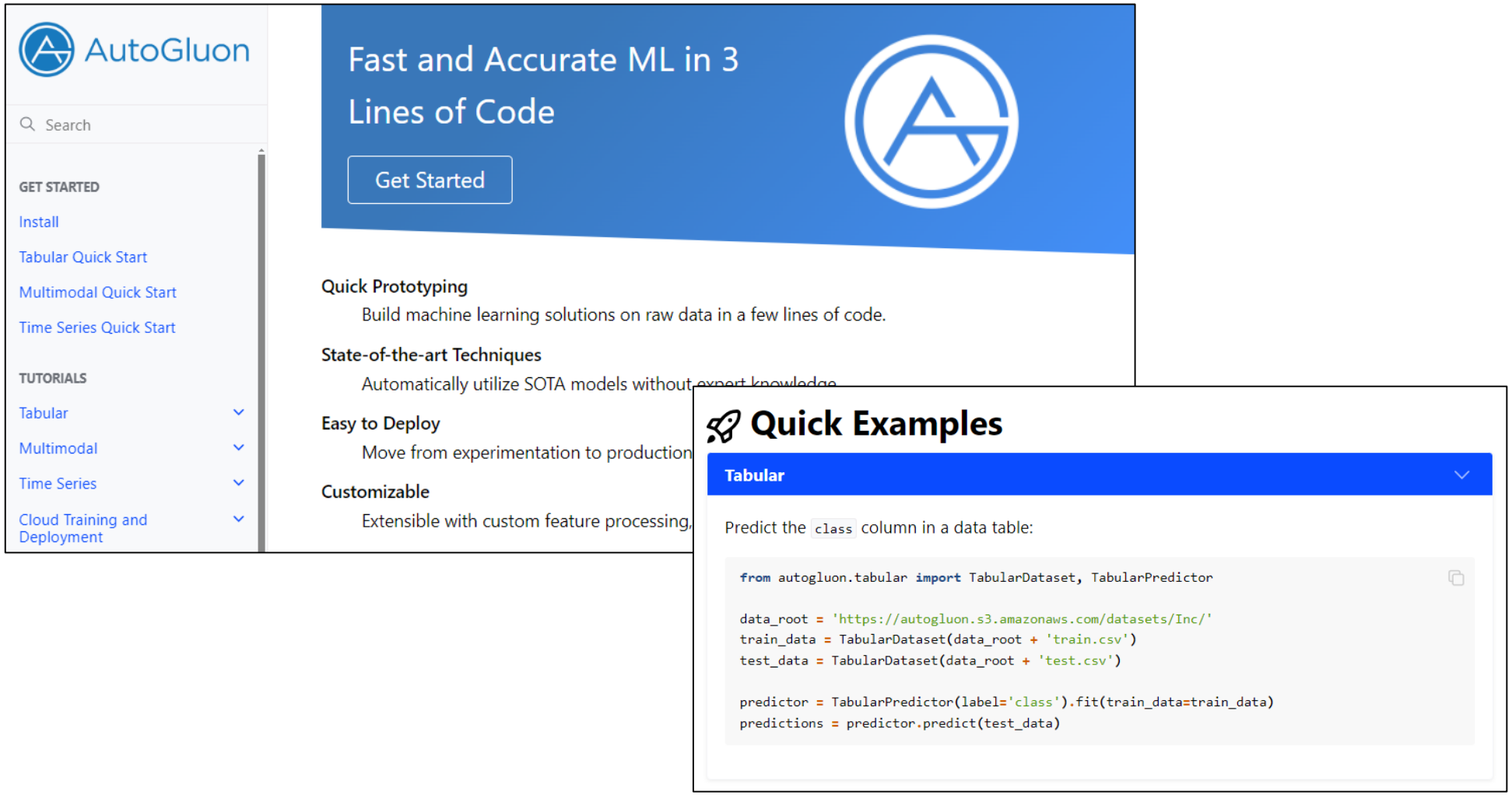
Example

```
>>> 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.

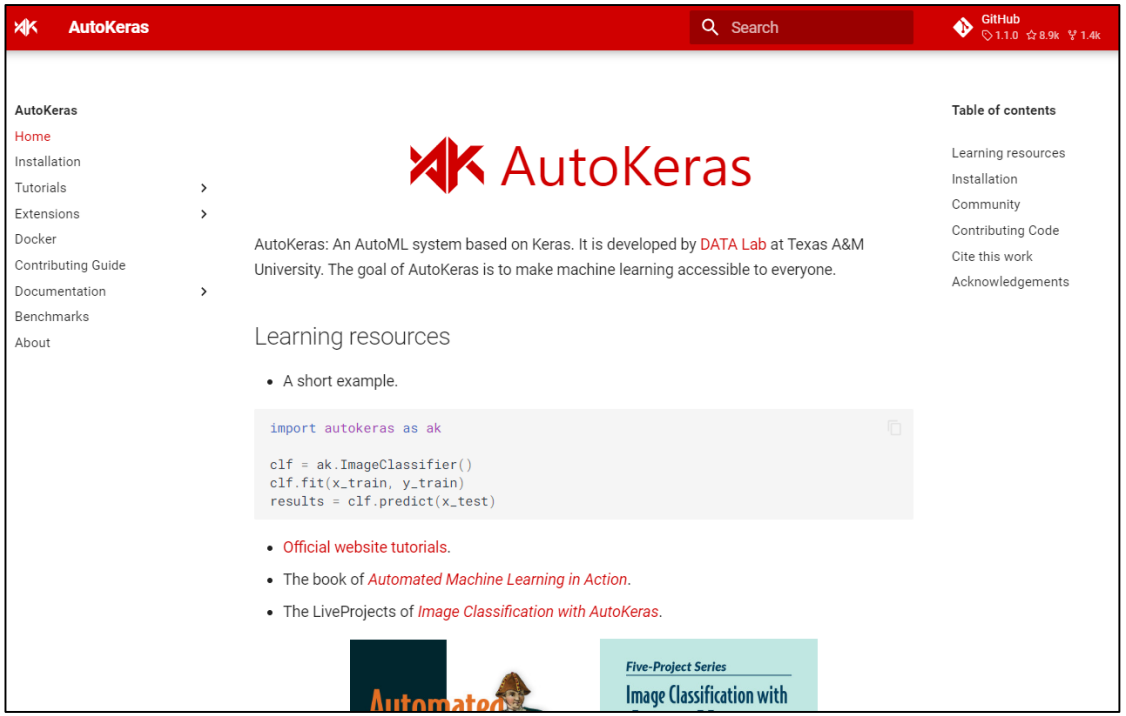
AutoGluon

https://auto.gluon.ai/



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

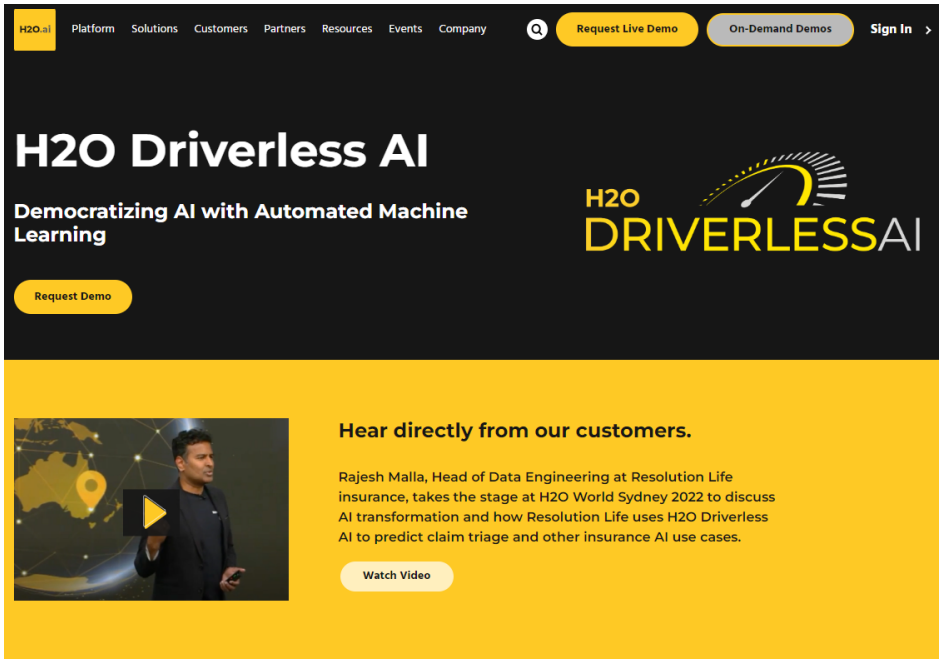
Structured Data Classification

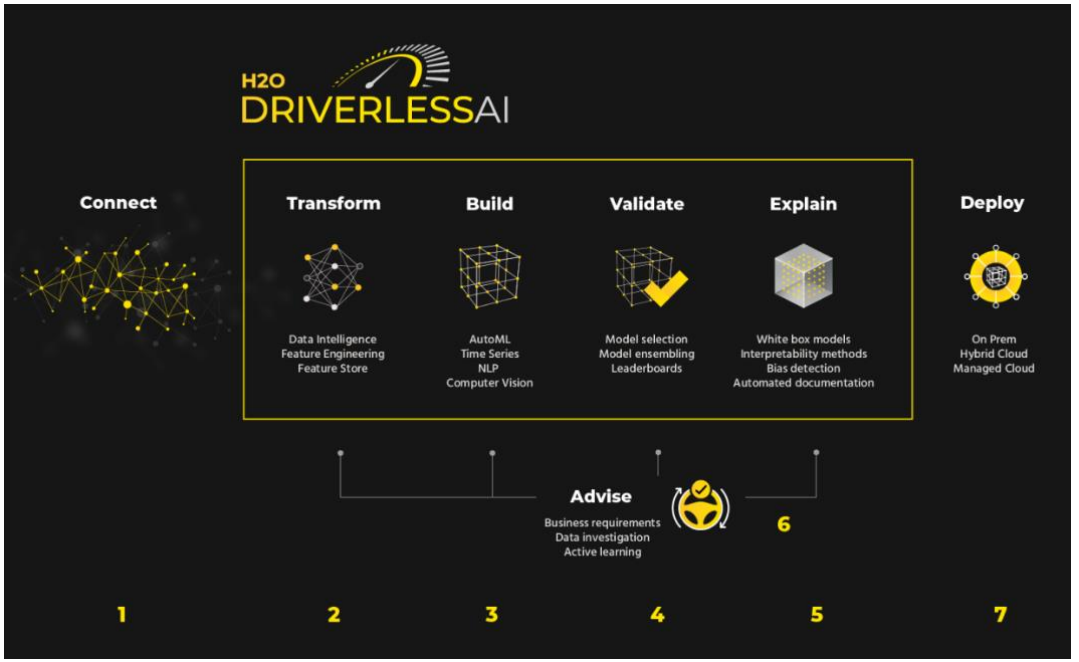
Structured Data Regression

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

H2O Driverless AI

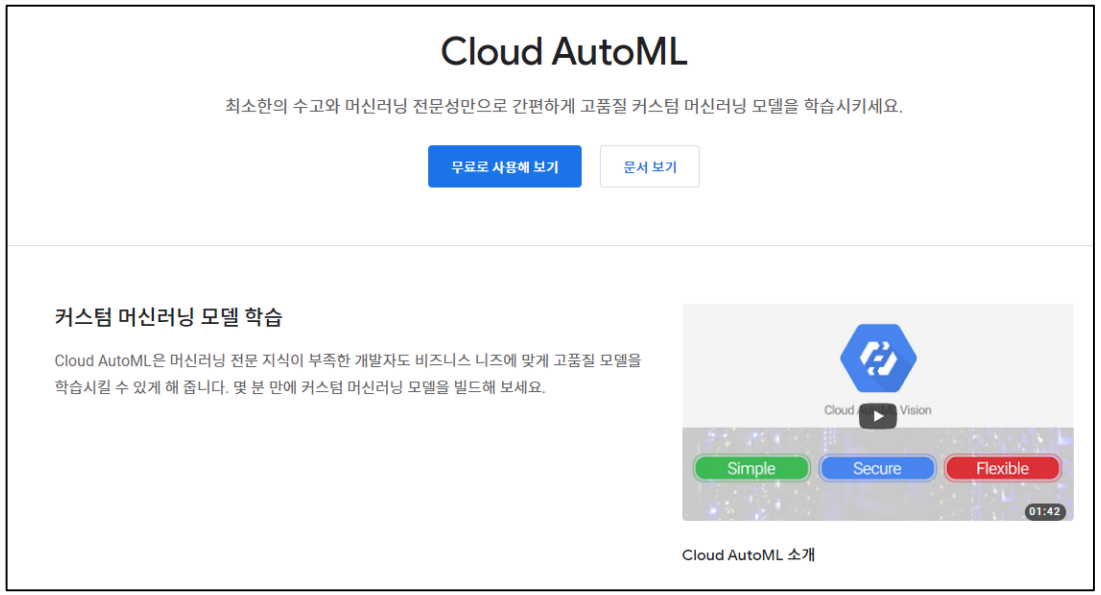
https://h2o.ai/platform/ai-cloud/make/h2o-driverless-ai/

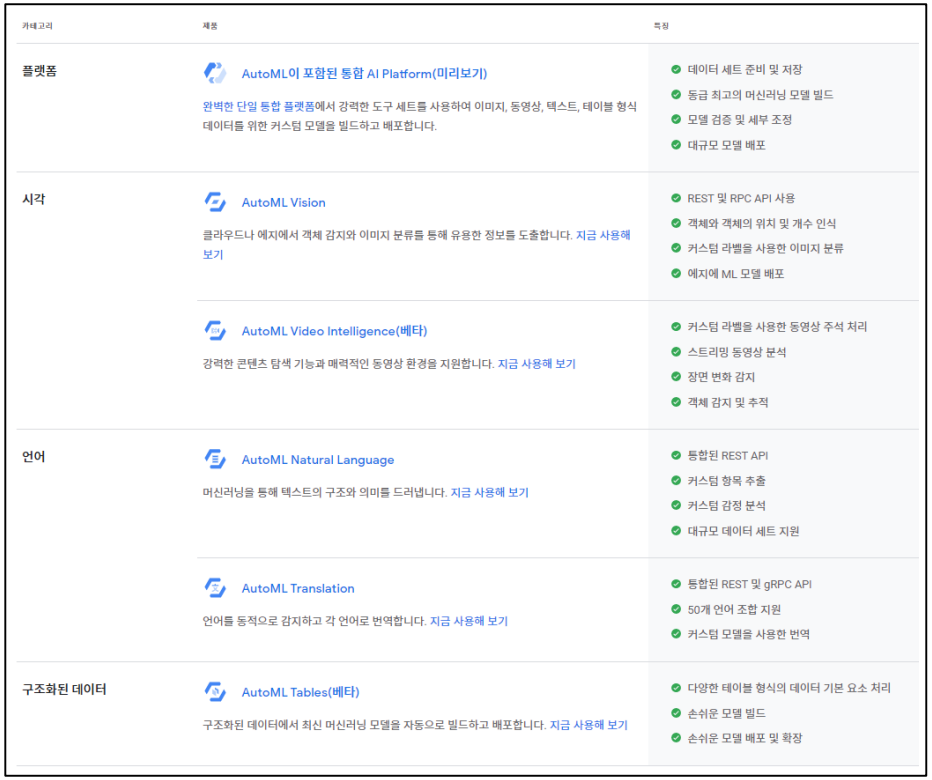




Google Cloud AutoML

https://cloud.google.com/automl





Tabular Foundation Model

- **Tabular Prior-data Fitted Network (TabPFN)**