LazyGrid

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LazyGrid is a python package providing an automatic, efficient and flexible implementation of complex machine learning pipeline generation and cross-validation.

Before fitting a model or a pipeline step, LazyGrid checks inside an internal SQLite database if the model has already been fitted. If the model is found, it won't be fitted again.

CHAPTER 1

Quick start

You can install LazyGrid along with all its dependencies from PyPI:

```
$ pip install -r requirements.txt lazygrid
```

CHAPTER 2

Source

The source code and minimal working examples can be found on GitHub.

2.1 Installation

You can install LazyGrid along with all its dependencies from PyPI:

```
$ pip install -r requirements.txt lazygrid
```

or from source code:

```
$ git clone https://github.com/glubbdubdrib/lazygrid.git
$ cd ./lazygrid
$ pip install -r requirements.txt .
```

LazyGrid is compatible with Python 3.5 and above.

2.2 Tutorial

LazyGrid has three main features:

- it can generate all possible pipelines given a set of steps (*Pipeline generation*) or all possible models given a grid of parameters (*Grid search*)
- it can compare the performance of a list of models using cross-validation and statistical tests (*Model comparison*), and
- it follows the memoization paradigm, avoiding fitting a model or a pipeline step twice.

2.2.1 Environment setup

Input data

In order to make each LazyPipeline transformer unique for different cross-validation splits, you must provide input data as DataFrame objects. The easiest way to transform numpy arrays into `DataFrame` data structures is the following:

```
import pandas as pd
...
X, y = ...
X = pd.DataFrame(X)
```

Organizing data sets and databases

If you are using more than one data set in your project, it is highly recommended to generate a hierarchy of database directories so that models fitted on different data sets can be easily identified:

```
import os
...
database_root_dir = "database"
data_set_name = "foo"
database_dir = os.path.join(database_root_dir, data_set_name)
if not os.path.isdir(database_dir):
    os.makedirs(database_dir)
```

This code will generate a directory structure as the following:

```
database
+-- foo
|   +-- database.sqlite
+-- baz
|   +-- database.sqlite
+-- ...
```

2.2.2 Model generation

Pipeline generation

In order to generate all possible pipelines given a set of steps, you should define a list of elements, which in turn are lists of pipeline steps, i.e. preprocessors, feature selectors, classifiers, etc. Each step could be either a `sklearn` object or a `keras` model.

Once you have defined the pipeline elements, the `generate_grid` method will return a list of models of type `lazygrid.lazy_estimator.LazyPipeline`.

The `LazyPipeline` class extends the `sklearn.pipeline.Pipeline` class by providing an interface to SQLite databases.

```
from sklearn.ensemble import RandomForestClassifier
from sklearn.svm import SVC
from sklearn.feature_selection import SelectKBest, f_classif
from sklearn.preprocessing import RobustScaler, StandardScaler
import lazygrid as lg

```

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```
preprocessors = [StandardScaler(), RobustScaler()]
feature_selectors = [SelectKBest(score_func=f_classif, k=1), SelectKBest(score_func=f_
↪classif, k=2)]
classifiers = [RandomForestClassifier(random_state=42), SVC(random_state=42)]

elements = [preprocessors, feature_selectors, classifiers]

list_of_models = lg.grid.generate_grid(elements)
```

Grid search

LazyGrid implements a useful functionality to emulate the grid search algorithm by generating all possible models given the model structure and its parameters.

In this case, you should define a dictionary of arguments for the model constructor and a dictionary of arguments for the fit method. The `generate_grid_search` method will return the list of all possible models.

The following example illustrates how to use this functionality to compare keras models with different optimizers and fit parameters.

```
import keras
from keras import Sequential
from keras.layers import Conv2D, MaxPooling2D, Flatten, Dense
from keras.utils import to_categorical
from sklearn.metrics import f1_score
from sklearn.datasets import load_digits
from sklearn.model_selection import StratifiedKFold
import lazygrid as lg
import numpy as np
import pandas as pd
from keras.wrappers.scikit_learn import KerasClassifier


# define keras model generator
def create_keras_model(optimizer):

    kmodel = Sequential()
    kmodel.add(Conv2D(32, kernel_size=(5, 5), strides=(1, 1),
                      activation='relu',
                      input_shape=x_train.shape[1:]))
    kmodel.add(MaxPooling2D(pool_size=(2, 2)))
    kmodel.add(Flatten())
    kmodel.add(Dense(1000, activation='relu'))
    kmodel.add(Dense(n_classes, activation='softmax'))

    kmodel.compile(loss=keras.losses.categorical_crossentropy,
                   optimizer=optimizer,
                   metrics=['accuracy'])
    return kmodel


# load data set
X, y = load_digits(return_X_y=True)
X = pd.DataFrame(X)

skf = StratifiedKFold(n_splits=10, shuffle=True, random_state=42)
```

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```
list_of_splits = [split for split in skf.split(x, y)]
train_index, val_index = list_of_splits[0]
x_train, x_val = x[train_index], x[val_index]
y_train, y_val = y[train_index], y[val_index]
x_train = np.reshape(x_train, (x_train.shape[0], 8, 8, 1))
x_val = np.reshape(x_val, (x_val.shape[0], 8, 8, 1))
n_classes = len(np.unique(y_train))
if n_classes > 2:
    y_train = to_categorical(y_train)
    y_val = to_categorical(y_val)


# cast keras model into sklearn model
kmodel = KerasClassifier(create_keras_model, verbose=1, epochs=0)

# define all possible model parameters of the grid
model_params = {"optimizer": ['SGD', 'RMSprop']}
fit_params = {"epochs": [5, 10, 20], "batch_size": [10, 20]}

# generate all possible models given the parameters' grid
models, fit_parameters = lg.grid.generate_grid_search(kmodel, model_params, fit_
↪params)
```

You will find the conclusion of this example in the *plot section*.

2.2.3 Model comparison

Optimized cross-validation

`LazyPipeline` objects can be extremely useful when a large number of machine learning pipelines need to be compared through cross-validation techniques.

In fact, once a pipeline step has been fitted, LazyGrid saves the fitted step into a SQLite database. Therefore, should the step be required by another pipeline, LazyGrid fetches the model that has already been fitted from the database.

This approach may boost the speed of time-consuming steps as recursive feature elimination techniques, voting classifiers or deep neural networks.

```
from sklearn.ensemble import RandomForestClassifier
from sklearn.svm import SVC
from sklearn.feature_selection import SelectKBest, f_classif, RFE
from sklearn.preprocessing import RobustScaler, StandardScaler
from sklearn.datasets import make_classification
import lazygrid as lg
import pandas as pd

X, y = make_classification(random_state=42)
X = pd.DataFrame(X)

preprocessors = [StandardScaler(), RobustScaler()]
feature_selectors = [RFE(RandomForestClassifier, n_features_to_select=10),
                     SelectKBest(score_func=f_classif, k=10)]
classifiers = [RandomForestClassifier(random_state=42), SVC(random_state=42)]

elements = [preprocessors, feature_selectors, classifiers]
```

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```
models = lg.grid.generate_grid(elements)

for model in models:
    scores = cross_validate(model, X, y, cv=10)
```

Statistical hypothesis tests

Once you have generated a list of models (or pipelines), LazyGrid provides friendly APIs to compare models' performances by using a cross-validation procedure and by analyzing the outcomes applying statistical hypothesis tests.

You can collect the cross-validation scores into a single list and call the `find_best_solution` method provided by LazyGrid. Such method applies the following algorithm: it looks for the model having the highest mean value over its cross-validation scores ("the best model"); it compares the distribution of the scores of each model against the distribution of the scores of the best model applying a statistical hypothesis test.

You can customize the comparison by modifying the statistical hypothesis test (it should be compatible with `scipy.stats`) or the significance level for the test.

```
...
scores = []
for model in models:
    score = cross_validate(model, X, y, cv=10)
    scores.append(score["test_score"])

best_idx, best_solutions_idx, pvalues = lg.statistics.find_best_solution(scores,
                                                                         ␣
↪test=mannwhitneyu,
                                                                          alpha=0.05)
```

2.2.4 Data set APIs

LazyGrid includes a set of easy-to-use APIs to fetch OpenML data sets (NB: OpenML has a database of more than 20000 data sets).

The `fetch_datasets` method allows you to smartly handle such data sets: it looks for OpenML data sets compliant with the requirements specified; for such data sets, it fetches the characteristics of their latest version; it saves in a local cache file the properties of such data sets, so that experiments can be easily reproduced using the same data sets and versions. You will find the list of downloaded data sets inside `./data/<datetime>-datalist.csv`.

The `load_openml_dataset` method can then be used to download the required data set version.

```
import lazygrid as lg

datasets = lg.datasets.fetch_datasets(task="classification", min_classes=2,
                                      max_samples=1000, max_features=10)

# get the latest (or cached) version of the iris data set
data_id = datasets.loc["iris"].did

x, y, n_classes = lg.datasets.load_openml_dataset(data_id)
```

2.3 Contributing to LazyGrid

First off, thanks for taking the time to contribute! :+1:

2.3.1 How Can I Contribute?

- Obviously source code: patches, as well as completely new files
- Bug report
- Code review

2.3.2 Coding Style

Notez Bien: All these rules are meant to be broken, **BUT** you need a very good reason **AND** you must explain it in a comment.

- Names (TL;DR): *module_name*, *package_name*, *ClassName*, *method_name*, *ExceptionName*, *function_name*, *GLOBAL_CONSTANT_NAME*, *global_var_name*, *instance_var_name*, *function_parameter_name*, *local_var_name*.
- Start names internal to a module or protected or private within a class with a single underscore (_); don't dunder (__).
- Use nouns for variables and properties names (*y = foo.baz*). Use full sentences for functions and methods names (*x = foo.calculate_next_bar(previous_bar)*); functions returning a boolean value (a.k.a., predicates) should start with the *is_* prefix (*if is_gargled(quz)*).
- Do not implement getters and setters, use properties instead. Whether a function does not need parameters consider using a property (*foo.first_bar* instead of *foo.calculate_first_bar()*). However, do not hide complexity: if a task is computationally intensive, use an explicit method (e.g., *big_number.get_prime_factors()*).
- Do not override *__repr__*.
- Use *assert* to check the internal consistency and verify the correct usage of methods, not to check for the occurrence of unexpected events. That is: The optimized bytecode should not waste time verifying the correct invocation of methods or running sanity checks.
- Explain the purpose of all classes and functions in docstrings; be verbose when needed, otherwise use single-line descriptions (note: each verbose description also includes a concise one as its first line). Be terse describing methods, but verbose in the class docstring, possibly including usage examples. Comment public attributes and properties in the *Attributes* section of the class docstring (even though PyCharm is not supporting it, yet); don't explain basic customizations (e.g., *__str__*). Comment *__init__* only when its parameters are not obvious. Use the formats suggested in the Google's style guide).
- Annotate all functions (refer to PEP-483) and PEP-484) for details).
- Use English for names, in docstrings and in comments (favor formal language over slang, wit over humor, and American English over British).
- Format source code using Yapf)'s style *"{based_on_style: google, column_limit=120, blank_line_before_module_docstring=true}"*
- Follow PEP-440) for version identification.
- Follow the Google's style guide) whenever in doubt.

2.4 Running tests

You can run all unittests from command line after having downloaded the source code from GitHub:

```
$ git clone https://github.com/glubbdubdrib/lazygrid.git
$ cd ./lazygrid
```

You can use either python:

```
$ python -m unittest discover
```

or coverage:

```
$ coverage run -m unittest discover
```

2.5 Database

`lazygrid.database`

2.6 Datasets

`lazygrid.datasets`

2.7 Grid

`lazygrid.grid`

2.8 Plotter

`lazygrid.plotter`

2.9 Statistics

`lazygrid.statistics`

2.10 Lazy Estimator

`lazygrid.lazy_estimator`

2.11 Authors

- Pietro Barbiero - Mathematical engineer - GitHub
- Giovanni Squillero - Professor of computer science at Politecnico di Torino - GitHub

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Version 2.0

Date January 2004

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- genindex
- modindex
- search