LazyGrid

Dec 13, 2019

User Guide

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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
```

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)
```

```
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.

```
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.

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.

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 <u>_____repr___</u>.
- 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 singleline 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., <u>_str_</u>). Comment <u>_init_</u> 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

```
lazygrid.database.drop_db(db_name: str) \rightarrow None
Drop database table if it exists.
```

Parameters db_name - Database name

Returns

Return type None

Examples

```
>>> import lazygrid as lg
>>>
>>> lg.database.drop_db(db_name="my-database.sqlite")
```

lazygrid.database.load_all_from_db(db_name: str, table_name: str = 'MODEL') → Op-

tional[Any]

Load all database items.

Parameters

- db_name Database name
- table_name Database table to load

Returns Query result

Return type Optional[Any]

2.6 Datasets

lazygrid.datasets

```
lazygrid.datasets.fetch_datasets (output_dir: str = './data', update_data: bool = False,

min_classes: int = 0, task: str = 'classification',

max_samples: int = inf, max_features: int = inf) \rightarrow pan-

das.core.frame.DataFrame
```

Load OpenML data sets compatible with the requirements.

Parameters

- output_dir Directory where the .csv file will be stored
- update_data If True it deletes cached data sets and downloads their latest version; otherwise it loads data sets as specified inside the cache
- min_classes Minimum number of classes required for each data set
- task Classification or regression
- max_samples Maximum number of samples required for each data set
- max_features Maximum number of features required for each data set

Returns Information required to load the latest version of each data set

Return type Dataframe

Examples

```
>>> import lazygrid as lg
>>>
>>> datasets = lg.datasets.fetch_datasets(task="classification", min_classes=2,_
→max_samples=1000, max_features=10)
>>> datasets.loc["iris"]
version
               45
            42098
did
              150
n_samples
                4
n_features
                 3
n_classes
Name: iris, dtype: int64
```

lazygrid.datasets.load_npy_dataset(path_x: str, path_y: str) -> (<class 'numpy.ndarray'>,

<class 'numpy.ndarray'>, <class 'int'>)

Load npy data set.

Parameters

- **path_x** Path to data matrix
- path_y Path to data labels

Returns Data matrix, data labels, and number of classes

Return type Tuple

Examples

```
>>> import os
>>> from sklearn.datasets import make_classification
>>> import numpy as np
>>> import lazygrid as lg
>>>
```

```
>>> x, y = make_classification(random_state=42)
>>>
>>> path_x, path_y = "x.npy", "y.npy"
>>> np.save(path_x, x)
>>> np.save(path_y, y)
>>>
>>>
>>>
x, y, n_classes = lg.datasets.load_npy_dataset(path_x, path_y)
```

Load OpenML data set.

Parameters

- data_id Data set identifier
- dataset_name Data set name

Returns Data matrix, data labels, and number of classes

Return type Tuple

Examples

```
>>> import lazygrid as lg
>>>
>>> x, y, n_classes = lg.datasets.load_openml_dataset(dataset_name="iris")
>>> n_classes
3
```

2.7 Grid

lazygrid.grid

lazygrid.grid.grid.generate_grid(elements: list, lazy: bool = True, **kwargs) → list Generate all possible combinations of sklearn Pipelines given the input steps.

Parameters

- elements List of elements used to generate the pipelines
- **lazy** If True it generates LazyPipelines objects; if False it generates standard sklearn Pipeline objects
- kwargs Keyword arguments to generate Pipeline objects

Returns List of pipelines

Return type list

Example

```
>>> 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
>>>
>>> preprocessors = [StandardScaler(), RobustScaler()]
>>> feature_selectors = [SelectKBest(score_func=f_classif, k=1),__
->> feature_selectors = [SelectKBest(score_func=f_classif, k=1),__
->> classifiers = [RandomForestClassifier(random_state=42), SVC(random_state=42)]
>>> elements = [preprocessors, feature_selectors, classifiers]
>>> pipelines = lg.grid.generate_grid(elements)
```

Generate all possible combinations of models.

Parameters

- model Model architecture
- model_params Model parameters. For each key the dictionary should contain a list of possible values
- fit_params Fit parameters. For each key the dictionary should contain a list of possible values

Returns Models and their corresponding fit parameters

Return type Tuple

Example

```
>>> import keras
>>> from keras import Sequential
>>> from keras.layers import Conv2D, MaxPooling2D, Flatten, Dense
>>> import lazygrid as lg
>>> from keras.wrappers.scikit_learn import KerasClassifier
>>>
>>> # define keras model generator
>>> def create_keras_model(input_shape, optimizer, n_classes):
       kmodel = Sequential()
. . .
       kmodel.add(Conv2D(32, kernel_size=(5, 5), strides=(1, 1), activation='relu
. . .
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
. . .
>>>
>>> # cast keras model into sklearn model
>>> kmodel = KerasClassifier(create_keras_model)
```

2.8 Plotter

lazygrid.plotter

```
lazygrid.plotter.plot_boxplots (scores: List, labels: List[str], file_name: str, title: str, out-
put_dir: str = './figures') -> dict
```

Generate and save boxplots.

Parameters

- **scores** List of scores to compare
- labels Name / identifier of each score list
- **file_name** Output file name
- title Figure title
- **output_dir** Output directory

Returns boxplot object

Return type Boxplot

Generate 3 plots: the test and training learning curve, the training samples vs fit times curve, the fit times vs score curve.

Parameters

- estimator (object type that implements the "fit" and "predict" methods) An object of that type which is cloned for each validation.
- **title** (*string*) Title for the chart.
- **X** (*array-like*, *shape* (*n_samples*, *n_features*)) Training vector, where n_samples is the number of samples and n_features is the number of features.
- **y** (array-like, shape (n_samples) or (n_samples, n_features), optional) Target relative to X for classification or regression; None for unsupervised learning.
- **axes** (array of 3 axes, optional (default=None)) Axes to use for plotting the curves.
- **ylim**(tuple, shape (ymin, ymax), optional) Defines minimum and maximum yvalues plotted.

- **cv**(*int*, *cross-validation* generator or an iterable, optional)-Determines the cross-validation splitting strategy. Possible inputs for cv are:
 - None, to use the default 5-fold cross-validation,
 - integer, to specify the number of folds.
 - CV splitter,
 - An iterable yielding (train, test) splits as arrays of indices.

For integer/None inputs, if y is binary or multiclass, StratifiedKFold used. If the estimator is not a classifier or if y is neither binary nor multiclass, KFold is used.

Refer User Guide for the various cross-validators that can be used here.

- n_jobs (int or None, optional (default=None)) Number of jobs to run in parallel. None means 1 unless in a joblib.parallel_backend context. -1 means using all processors. See Glossary for more details.
- train_sizes (array-like, shape (n_ticks,), dtype float or int) - Relative or absolute numbers of training examples that will be used to generate the learning curve. If the dtype is float, it is regarded as a fraction of the maximum size of the training set (that is determined by the selected validation method), i.e. it has to be within (0, 1]. Otherwise it is interpreted as absolute sizes of the training sets. Note that for classification the number of samples usually have to be big enough to contain at least one sample from each class. (default: np.linspace(0.1, 1.0, 5))

2.9 Statistics

lazygrid.statistics

lazygrid.statistics.confidence_interval_mean_t (x: numpy.ndarray, cl: float = 0.05) \rightarrow

List Compute the confidence interval of the mean from sample data.

Parameters

- **x** Sample
- **cl** Confidence level

Returns confidence interval

Return type List

Examples

```
>>> import numpy as np
>>> import lazygrid as lg
>>>
    np.random.seed(42)
>>> x = np.random.normal(loc=0, scale=2, size=10)
>>> confidence_level = 0.05
>>>
lg.statistics.confidence_interval_mean_t(x, confidence_level)
[-0.13829578539063092, 1]
```

Notes

You should use the t distribution rather than the normal distribution when the variance is not known and has to be estimated from sample data.

When the sample size is large, say 100 or above, the t distribution is very similar to the standard normal distribution. However, with smaller sample sizes, the t distribution is leptokurtic, which means it has relatively more scores in its tails than does the normal distribution. As a result, you have to extend farther from the mean to contain a given proportion of the area.

lazygrid.statistics.find_best_solution (solutions: list, test: Callable = <function mannwhitneyu>, alpha: float = 0.05, **kwargs) -> (<class 'int'>, <class 'list'>, <class 'list'>)

Find the best solution in a list of candidates, according to a statistical test and a significance level (alpha).

The best solution is defined as the one having the highest mean value.

Parameters

- **solutions** List of candidate solutions
- test Statistical test
- **alpha** Significance level
- kwargs Keyword arguments required by the statistical test

Returns

- the position of the best solution inside the candidate input list;
- the positions of the solutions which are not separable from the best one;
- the list of p-values returned by the statistical test while comparing the best solution to the other candidates

Return type Tuple

Examples

```
>>> from sklearn.linear model import LogisticRegression, RidgeClassifier
>>> from sklearn.ensemble import RandomForestClassifier
>>> from sklearn.datasets import make_classification
>>> from sklearn.model_selection import cross_val_score
>>> import lazygrid as lg
>>>
>>> x, y = make_classification(random_state=42)
>>>
>>> model1 = LogisticRegression(random_state=42)
>>> model2 = RandomForestClassifier(random_state=42)
>>> model3 = RidgeClassifier(random_state=42)
>>> model_names = ["LogisticRegression", "RandomForestClassifier",
↔ "RidgeClassifier"]
>>>
>>> score1 = cross_val_score(estimator=model1, X=x, y=y, cv=10)
>>> score2 = cross_val_score(estimator=model2, X=x, y=y, cv=10)
>>> score3 = cross_val_score(estimator=model3, X=x, y=y, cv=10)
>>>
>>> scores = [score1, score2, score3]
>>> best idx, best solutions idx, pvalues = lq.statistics.find best
⇔solution(scores)
```

```
>>> model_names[best_idx]
'LogisticRegression'
>>> best_solutions_idx
[0, 2]
>>> pvalues #doctest: +ELLIPSIS
[0.4782..., 0.0360..., 0.1610...]
```

2.10 Lazy Estimator

lazygrid.lazy_estimator

A LazyPipeline estimator.

A lazy pipeline is a sklearn-like pipeline that follows the memoization paradigm. Once the pipeline has been fitted, its steps are pickled and stored in a local database. Therefore, when the program starts again, the pipeline will fetch its fitted steps from the database and will skip the fit operation.

Parameters

- **steps** 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.
- database Used to cache the fitted transformers of the pipeline. It is the path to the database directory. Caching the transformers is advantageous when fitting is time consuming.
- **verbose** (*bool*, *default=False*) If True, the time elapsed while fitting each step will be printed as it is completed.

named_steps

Read-only attribute to access any step parameter by user given name. Keys are step names and values are steps parameters.

Type bunch object, a dictionary with attribute access

See also:

sklearn.pipeline.Pipeline

Examples

```
>>> from sklearn import svm
>>> from sklearn.datasets import make_classification
>>> from sklearn.feature_selection import SelectKBest
>>> from sklearn.feature_selection import f_regression
>>> from lazygrid.lazy_estimator import LazyPipeline
>>> import pandas as pd
>>> # generate some data to play with
>>> X, y = make_classification(
... n_informative=5, n_redundant=0, random_state=42)
>>> X = pd.DataFrame(X)
>>> # ANOVA SVM-C
>>> anova_filter = SelectKBest(f_regression, k=5)
>>> clf = svm.SVC(kernel='linear')
```

```
>>> anova_svm = LazyPipeline([('anova', anova_filter), ('svc', clf)])
>>> # You can set the parameters using the names issued
>>> # For instance, fit using a k of 10 in the SelectKBest
>>> # and a parameter 'C' of the svm
>>> anova_svm.set_params(anova_k=10, svc_C=.1).fit(X, y)
Pipeline(steps=[('anova', SelectKBest(...)), ('svc', SVC(...))])
>>> prediction = anova_svm.predict(X)
>>> anova_svm.score(X, y)
0.83
>>> # getting the selected features chosen by anova_filter
>>> anova_svm['anova'].get_support()
array([False, False, True, True, False, False, True, True, False,
      True, False, True, True, False, True, False, True, True,
      False, False])
>>> # Another way to get selected features chosen by anova_filter
>>> anova_svm.named_steps.anova.get_support()
array([False, False, True, True, False, False, True, True, False,
      True, False, True, True, False, True, False, True, True,
      False, False])
>>> # Indexing can also be used to extract a sub-pipeline.
>>> sub_pipeline = anova_svm[:1]
>>> sub_pipeline
Pipeline(steps=[('anova', SelectKBest(...))])
>>> coef = anova_svm[-1].coef_
>>> anova_svm['svc'] is anova_svm[-1]
True
>>> coef.shape
(1, 10)
>>> sub_pipeline.inverse_transform(coef).shape
(1, 20)
```

fit (X: pandas.core.frame.DataFrame, y: Iterable = None, **fit_params)
Fit the model

Fit all the transforms one after the other and transform the data, then fit the transformed data using the final estimator.

Parameters

- X Training data. Must fulfill input requirements of first step of the pipeline.
- y Training targets. Must fulfill label requirements for all steps of the pipeline.
- ****fit_params** (dict of string -> object) Parameters passed to the fit method of each step, where each parameter name is prefixed such that parameter p for step s has key s_p.

Returns This estimator

Return type self

2.11 Authors

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

2.12 Apache License

Version 2.0 Date January 2004 URL http://www.apache.org/licenses/

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