Simulation studies on Python using sstudy package with SQL databases as storage

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Abstract

Performance assessment is a key issue in the process of proposing new machine learning/statistical estimators. A possible method to complete such task is by using simulation studies, which can be defined as the procedure of estimating and comparing properties (such as predictive power) of estimators (and other statistics) by averaging over many replications given a true distribution; i.e.: generating a dataset, fitting the estimator, calculating and storing the predictive power, and then repeating the procedure many times and finally averaging over the stored predictive powers. Given that, in this paper, we present sstudy: a Python package designed to simplify the preparation of simulation studies using SQL database engines as the storage system; more specifically, we present its basic features, usage examples and references to the its documentation. We also present a short statistical description of the simulation study procedure with a simplified explanation of what is being estimated by it, as well as some examples of applications.

Keywords: simulation study, machine learning, python, sstudy

1 Introduction

One important aspect of proposing new machine learning/statistical estimators and methods is the performance test phrase. A possible way to access such performance is by simulation studies, which can be defined as the procedure of estimating and comparing properties (such as predictive power) of estimators (and other statistics) by averaging over many replications given a true distribution; i.e.: generating a dataset, then fitting the estimator, calculating and storing the predictive power, and then repeating the procedure many times and finally averaging over the predictive powers across repetitions.

In this paper, we present a Python package called sstudy which is designed to simplify their preparation and execution using SQL database engines. We also present a short statistical description of the simulation study procedure, as well as some examples of applications.

1.1 Terminology

Given the mixed audience nature of this paper, we use the following terms interchangeably:

- Train model, fit model to data.
- Dataset, sample.
- Number of instances, sample size.
- Dataset generator, true distribution, data generating function.
- Loss, decision criteria.

1 For a more extensible presentation on simulations studies themselves, see Morris, White, and Crowther [2].
1.2 Article organization

The rest of this paper is organized as follows: in section 2, we present a short introduction on simulation studies, with a short statistical notation of what is being estimated by them and some examples of applications. In section 3, we present a short introduction on sstudy package, with examples of basic usage as well as presenting its features and usage examples available in its documentation. Finally, section 4 concludes the paper.

2 On simulation studies:

The process of a simulation study consists of varying some aspects of the data generating function, the estimating model and estimating its performance by averaging over distinct random seeds for the data generator; i.e., estimating:

\[ E_{D \in \mathbb{D}_P} [\text{loss}(M_k(D), D)] \]

where

- \( P \) are the parameters of the data generating function (e.g.: distribution parameters, number of instances, etc).

- \( k \) are model parameters (e.g.: whether you are using a linear regression, a lasso or a ridge, and if a lasso/ridge, what is its tuning parameter, etc).

So, in other words, a simulation study is a repetition of the following procedure many times followed by averaging over the results: generate a dataset \( D \) from a ground truth distribution \( \mathbb{D}_P \), train a model \( M_k \) using this dataset and then evaluate the loss.

Note however, that in order to avoid overfitting, one must train and evaluate the loss on distinct partitions of the dataset \( D \). Algorithm 1 summarizes the procedure.

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**Algorithm 1** Simulation study procedure

**Input:** dataset generator \( \mathbb{D}_P \), model \( M_k \), number of desired simulations \( n_{\text{sim}} \).

**Output:** loss over simulations.

1. for \( i \in \{1, \ldots, n_{\text{sim}}\} \) do
2. Generate dataset \( D_{\text{train}} \) and \( D_{\text{test}} \) from \( \mathbb{D}_P \).
3. Train model \( M_k \) using \( D_{\text{train}} \); i.e. calculate \( M_k(D_{\text{train}}) \).
4. Evaluate loss \( (M_k(D_{\text{train}}), D_{\text{test}}) \) and store it on \( L_i \)
5. end for
6. Return the mean of \( L \).

2.1 Example with a simple regression

Suppose that we want to compare the performance of ordinary least squares with the performance of a lasso with data being generated from a Gaussian linear regression: e.g.: each dataset contains 100 instances \((X_1, X_2, \ldots, X_{100})\), with each instance arising independently from a \( Y | X \sim \text{Gaussian}(X \beta, \sigma) \). \( X \sim \text{Multivariate Gaussian}(0, 2I) \).

In other to proceed with the evaluation, one must note first that there are many possibilities that we could setup here in order to test the estimators performance: we can compare the estimated values of \( \mu = X \beta \) or compare directly the estimated \( y \)'s. Moreover, we can also choose from a wide range of loss criteria\(^3\) like the mean squared error, mean absolute error, etc.

A second point to notice here is that one might be tempted to generate a single train dataset

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\(^2\) Note that, in some cases, however it is not necessary to generate a test dataset because a dataset might not be necessary at all in the evaluation phrase; e.g.: if you want to compare the estimated parameter directly to the true model parameter.

\(^3\) Without loss of generality, you can also work with utility, score and other decision criteria.
data. In this case however, we would be affected by random chance and would be unable to conclude with certainty which model bests adjust to the data: maybe model A is better for this true distribution, but by chance it happened to obtain a bad fit this specific dataset that was generated.

If however, we try to solve this problem by means of increasing the train dataset size, then we fall into another problem: we would be concluding which model better fits a large sample size instead of perceiving their behaviour on smaller samples\(^4\), but in the real world, we do not have access to an infinite amount of data.

The solution given by a simulation study is to repeat such a procedure many times to the point that in the long run, we are able to distinguish which model is the best for this true distribution and this decision criteria even in the presence of small datasets.

In Table 1, we present the results for such a simulation experiment (in parenthesis we present the standard error of measurement of the simulation study, note that if you increase the number of simulations, this number will tend to zero). Its source code is available at the sstudy package documentation (https://sstudy.marcoinacio.com/).

Table 1: Results for a simulation experiment using a Gaussian linear regression as dataset generator.

| data distribution | n. of instances | method | score   |
|-------------------|------------------|--------|---------|
| complete          | 100              | lasso  | 0.803 (0.035) |
|                   |                  | ols    | 0.838 (0.008) |
|                   | 1000             | lasso  | 0.856 (0.011) |
|                   |                  | ols    | 0.834 (0.010) |
|                   | 10000            | lasso  | 0.842 (0.016) |
|                   |                  | ols    | 0.825 (0.012) |
| sparse            | 100              | lasso  | 0.608 (0.073) |
|                   |                  | ols    | 0.660 (0.022) |
|                   | 1000             | lasso  | 0.747 (0.049) |
|                   |                  | ols    | 0.702 (0.022) |
|                   | 10000            | lasso  | 0.688 (0.040) |
|                   |                  | ols    | 0.695 (0.021) |

2.2 Another example: pvalues of hypothesis tests

Simulation studies can also be used to compare the hypothesis testing methods (see Almeida Inácio, Izbicki, and Gyires-Tóth [3] and Almeida Inácio, Izbicki, and Stern [4], for instance). In this case, two important criteria arises: the uniformity of the test under the null hypothesis and the test power under the alternative hypothesis.

Given a dataset \(D_{\text{train}}\) (i.e.: a sample \((X_1, X_2, ..., X_n)\)) with each instance coming independently from a Gaussian \((\mu = 2, 1)\), we could, for instance, compare the tests type I error rate of method A and B under the null hypothesis \(\mu = 2\) and compare the test power of such methods under the alternative hypothesis \(\mu = 3.5\).

Additionally, we could change the true distribution to something other than a Gaussian to verify how that affects the type I error and the test power.

\(^4\) Note that models that have terrible behaviour on small datasets, might get increasingly better as the sample size increases (i.e.: bad estimators might be consistent). An example would be the estimator \(\sum_{i=1}^{n} x_i / (n - 10000)\) which is generally bad for small samples but equals to the empirical mean as \(n\) approaches infinity.
2.3 Non-deterministic estimators

For neural networks and other non-deterministic estimators, in general, we also randomize the initialization parameters of the estimator.

In this case, suppose that the method becomes deterministic given a vector of parameters $\beta$, we would then be estimating:

$$E_{D \in D} \left[ \text{loss} \left( M_{\{k, \beta\}}, D \right) \right]$$

Therefore, the non-determinism of the method would be “averaged out” after a large number of simulations and the same conclusions would follow as was previously done.

3 The sstudy package

In this section, we present the basic usage of the package as well as some of its features.

3.1 Basic usage

The recommended design of an experiment using the package is by having it separated in 3 files:

- A file for database structure where we declare the variables to be stored in the SQL database and their respective types (see Listing 1).
- A file for running the simulations where we declare the list of parameters to be simulated, as well as the simulation script itself (see Listing 2).
- A file to explore/plot the results which can be exported directly into a pandas.DataFrame (see Listing 3).

To see the complete source code of listings 1, 2 and 3, see the example folder distributed together with the package, which is also available at: https://github.com/randommm/sstudy/tree/master/example.

3.2 Main features and documented examples

In the package documentation available at https://sstudy.marcoinacio.com/, we present the following features and examples:

- Support to sqlite, postgresql, mysql and cockroachdb (and, at least in principle, any additional dataset supported by peewee).
- Automatic randomization of executions.
- Optional filter of undesired simulation options.
- Prevention of SQL server disconnect failures: waits for availability of the server again so that long simulation calculations are not lost.

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5 e.g.: for neural networks, using random Xavier [5] or Kaiming [6] initializations.
6 For neural networks, that would be the initial value of its neurons.
Listing 2: Part of the simulation execution file

to_sample = dict(
    data_distribution = ["complete", "sparse"],
    no_instances = [100, 1000],
    method = ["ols", "lasso"],
)

def func(
    data_distribution,
    no_instances,
    method,
):
    x = stats.norm.rvs(0, 2, size=(no_instances + 10000, 10))
    beta = stats.norm.rvs(0, 2, size=(10, 1))
    eps = stats.norm.rvs(0, 5, size=(no_instances + 10000, 1))
    if data_distribution == "complete":
        y = np.matmul(x, beta) + eps
    elif data_distribution == "sparse":
        y = np.matmul(x[:,:5], beta[:5]) + eps
    else:
        raise ValueError

    y_train = y[:no_instances]
    y_test = y[no_instances:]
    x_train = x[:no_instances]
    x_test = x[no_instances:]

    start_time = time.time()
    if method == 'ols':
        reg = LinearRegression()
    elif method == 'lasso':
        reg = Lasso(alpha=0.1)
    reg.fit(x_train, y_train)
    score = reg.score(x_test, y_test)
    elapsed_time = time.time() - start_time

    return dict(
        score = score,
        elapsed_time = elapsed_time,
    )

do_simulation_study(to_sample, func, db, Result,
max_count=no_simulations)

Listing 3: Part of the simulation study results exploration file

import pandas as pd
...
df = pd.DataFrame(list(Result.select().dicts()))
df.groupby(["data_distribution", "no_instances", "method"]).mean()
Automatic handling of binary data: whenever a dataset field is a `BlobField`, invokes the “binarizer” `pickle.dumps` automatically. This allows the user to store whole arrays or large class instances as results into the SQL database.

- Hints on exploring the results using `pandas` package.

4 Conclusion

In this short paper, we have presented a Python package called `sstudy`, designed to simplify the preparation of simulation studies; we presented its basic features, usage examples and references to the its documentation. Moreover, we also presented a short statistical description of the simulation study procedure.

5 Acknowledgments

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