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A Comparative study of data splitting algorithms for machine learning model selection

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Abstract

Data splitting is commonly used in machine learning to split data into a train, test, or validation set. This approach allows us to find the model hyper-parameter and also estimate the generalization performance. In this research, we conducted a comparative analysis of different data partitioning algorithms on both real and simulated data. Our main objective was to address the question of how the choice of data splitting algorithm can improve the estimation of the generalization performance. Data splitting algorithms used in this study were variants of k-fold, Kennard-Stone, SPXY (sample set partitioning based on joint x-y distance), and random sampling algorithm. Each algorithm divided the data into two subset, training/validation. The training set was used to fit the model and validation for the evaluation. We then analyzed the different data splitting algorithms based on the generalization performances estimated from the validation and the external test set.

From the result, we noted that the important determinant for a good generalization is the size of the dataset. For all the data sample methods applied on small data set, the gap between the performance estimated on the validation and test set was significant. However, we noted that the gap reduced when there was more data in training or validation. Too many or few data in the training set can also lead to bad model performance. So it is importance to have a reasonable balance between the training/validation set sizes. In our study, KS and SPXY was the splitting algorithm with poor model performance estimation. Indeed these methods select the most representative samples to train the model, and poor representative samples are left for model performance estimation.

Keywords: K-fold, cross-validation, Kennard-Stone algorithm, data splitting, bootstrap, overfitting, SPXY

Sammanfattning

Datapartitionering används vanligtvis i maskininlärning för att dela data i en tränings, test eller valideringsuppsättning. Detta tillvägagångssätt gör det möjligt för oss att hitta hyperparametrar för modellen och även uppskatta generaliseringsprestanda. I denna forskning genomförde vi en jämförande analys av olika datapartitionsalgoritmer på både verkliga och simulerade data. Vårt huvudmål var att undersöka frågan om hur valet avdatapartitioneringsalgoritm kan förbättra uppskattningen av generaliseringsprestanda.
Datapartitioneringsalgoritmer som användes i denna studie var varianter av k-faldig korsvalidering, Kennard-Stone (KS), SPXY (partitionering baserat på gemensamt x-y-avstånd) och bootstrap-algoritm. Varje algoritm användes för att dela upp data i två olika datamängder: tränings- och valideringsdata. Vi analyserade sedan de olika datapartitioneringsalgoritmerna baserat på generaliseringsprestanda uppskattade från valideringen och den externa testuppsättningen.

Från resultatet noterade vi att det avgörande för en bra generalisering är storleken på data. För alla datapartitioneringsalgoritmer som använts på små datamängder var klyftan mellan prestanda uppskattad på valideringen och testuppsättningen betydande. Vi noterade emellertid att gapet minskade när det fanns mer data för träning eller validering. För mycket eller för litet data i träningsuppsättningen kan också leda till dålig prestanda. Detta belyser vikten av att ha en korrekt balans mellan storlekarna på tränings- och valideringsmängderna. I vår studie var KS och SPXY de algoritmer med sämst prestanda. Dessa metoder väljer de mest representativa instanserna för att träna modellen, och icke-representativa instanser lämnas för uppskattning av modellprestanda.

Nyckelord: k-faldig korsvalidering, korsvalidering, Kennard-Stone-algoritm, datapartitionering, bootstrap, överanpassning, SPXY

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Contents

1 Introduction

This chapter presents a general background and problem formulation. Also, the organization of the thesis work is presented as well as objectives and purpose.

1.1 Background

Machine learning algorithms aim to extract knowledge from data and produce viable prediction models. One of the main goal is to build computational models with high prediction and generalization capabilities [19]. The generalization ability depends on the model complexity. The complexity of a machine learning model depends on his hyper-parameters. A model with high complexity can have a risk of over-fitting. However, data splitting into training and validation sets can help to find the most efficient set of model parameter(s), which has a correct balance between the model generalization capabilities and his complexity. The training data is used to fit the model with the parameters [16]. The model can see this data and learn from it. On the other hand, the validation set used to challenge the model. The validation used to evaluate the model fitted with the trained data while tuning the model's hyperparameters. This is the model selection procedure [20].

Recent research has shown that the validation set is not always enough to measure the model's performance. Westerhuis et al. [21] have demonstrated that cross-validation can give an over-optimistic result. The study of Harrington et al. [8] proved that having only training and validation sets could also give a wrong estimation of model performance. These studies highlight the need to have another set. This external test set allows us to evaluate the generalization performance of the model on unseen data. Machine learning model validation process can be illustrated with flowchart in figure 1.1 [22]. However, even with the process described in (Fig. 1), it is still challenging to have an external data set with the same distribution as data in real-world applications. Indeed, the data structure, in real-world applications, is most of the time unknown in advance. Also, many other factors can affect the model generalization performance. The size of the different data sets, training validation, test set, and the data splitting

algorithm can impact the model.

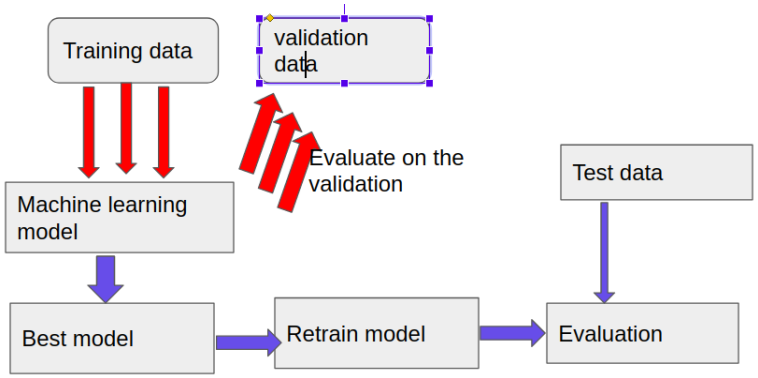

Figure 1.1: A model selection general flowchart. " arrows in red color is the validation flow and blue arrows the final training and evaluation with external test flow " source: [22].

1.2 Problem

Our study centered on three categories of data splitting algorithms: random splitting, cross-validation, and rational splitting algorithm. Random selection algorithms randomly select a set of samples a validation, and the remaining ones are used to fit the model. This process can be repeated many times. The selection can be with or without replacement. The bootstrap algorithm proposed by Efron et al. [8] is an example of a random splitting algorithm for our analysis. On the other hand, rational splitting algorithms select samples base on the similarity between the data point or the data distribution. The objective is to select the most representative sample for the training set. Kennard-Stone algorithm was used in our study as an example rational splitting algorithm. Cross-validation algorithm is described in the next chapter.

Most of the data splitting algorithms have a parameter that must be chosen wisely—for example, the parameter k for k-fold cross-validation or the number of repetitions for random splitting. The different splitting algorithms used in our study are fully described in the literature. Daszykowski et al. [1] proposed a report of different rational splitting algorithms. The different effects of KS algorithm have been studied by Puzyn et al. [23]. However, to our knowledge, no comparative analysis of the three data splitting categories has

been done before. No previous study has evaluated the impact of the data splitting parameter on a machine learning model for a regression problem. Therefore, in this study, we analyzed three categories of data splitting algorithms. For each algorithm, we investigated the impact of his parameter on the model generalization performance. These methods include a k-fold CV, bootstrapping [8], SPXY, and KS.

1.3 Purpose

Splitting the data into different sets is technique commonly used in machine learning. The data is usually divided into training and validation set in order to train and find the model hyperparameters (model selection) and estimate the model prediction error or accuracy. What about the algorithm used to split the data set? What is the impact of the algorithm on model accuracy or error? Some data splitting algorithms also have a parameter that needs to be optimized. For example, the parameter k for k-fold cross-validation or the number of repetitions for random splitting. This leads us to the research question of how the choice of data splitting algorithm for the training/validation set can improve the estimation of the generalization performance. The purpose of the study is to answer this research question by assuming the hypothesis that generalization performance depends on the splitting algorithm used for the model selection.

Our research centered on the case where the objective of the machine learning model is to have a high correlation score. The model prediction on validation and test set are then compared based on the Pearson correlation score. The test set was unseen by the model during the training. To our knowledge, the research question proposed here has not been addressed before. [14] conducted a comparative analysis of different k-fold cross-validations.

Dobbin and Simon [4] proposed an algorithm for train set size planning. No previous studies went deeper to analyze the impact of sample splitting parameters on the machine learning model's generalization performance.

1.4 Goal

This work aims to see whether data splitting influences the external predictivity of the machine learning model. This study's conclusion can give researchers and machine learning engineers valuable insight into whether it is worthwhile to fine-tune different splitting algorithms and select the best one and his corresponding parameter when implementing a machine learning system. Our study is part of a research project at the Institute of Chemistry of Nice and the long term goal is to implement a system able to predict the effect molecules on human emotion with high accuracy.

1.4.1 Benefits, Ethics and Sustainability

Through this study, a reader can learn more about the reasoning for selecting a specific data splitting algorithm when implementing machine learning.

In terms of Ethics, the real data used in this study are collected from the Dream olfaction challenge website, which is publicly available and does not contain any sensitive data. It has been entirely anonymized to prevent any unnecessary risks to individuals whose data is being used. According to the General Data Protection Regulation (GDPR) [15], anonymized data can be used for research purposes as it does not expose the individual personal data.

When it comes to the sustainability aspects, all research areas need to contribute to the United Nations' sustainable development goals[18]. Our long-term goal will contribute to achieving the responsible consumption and production goal of the UN. Predicting the effect of molecules will improve the way perfumes are created. It will then limit the waste of chemical substances. Indeed Perfumers usually make many chemical tests to produce fragrance with the desired odor and effect. Some chemical substances are thrown into the environment.

1.5 Methodology

The research started by collecting previous studies nearly matching our research topic. We explored different data splitting approaches. The purpose was to see which splitting will improve the model prediction on the unseen data set. The

research question is being answered with a quantitative method and a empirical research approach.

1.6 Delimitations

We have identified the following limitations of the work.

- We used regression problem and one machine learning algorithm, random forest, to answer our research question. This means that our study's outcome may be different if it was a classification problem or another machine learning algorithm.
- Our study focus on three category of splitting algorithm, there is a possibility that by evaluating more splitting algorithms, another result could be found
- The machine learning algorithm's performance can also be influenced by some factors such as computational resources. However, efficiency is not evaluated in this thesis as it is not the scope of our study.

1.7 Outline

The remaining part of the report is structured as follows; in chapter two, we present the different splitting algorithms chosen for our study. Chapter three focuses on our research methodology. The result of our implementation is shown in chapter four. Finally, discussions and future work suggestions are presented in chapter five..

2 Extended Background

This section presents details explanation of the different splitting algorithms used in our work.

2.1 Data Splitting Method

2.1.1 Cross-Validation (CV)

Based on our literature review, a cross-validation algorithm is a method commonly used in machine learning. Data is split into k different parts. For each iteration, k-1 parts are used to train the model and the remaining part as a validation set. The process is iterated according to the number of fold. The generalization performance of the model is the average of the estimated scores. The model parameter with the best averaged predictive score is used as the optimal. This technique is referred to as K-fold cross-validation algorithm. More details description can be found in [10]

2.1.2 Bootstrap

The bootstrap algorithm is a method of resampling data. It is assessing the statistics and properties of a potential distribution without actually knowing its distribution [18]. The work of Kohavi [19] has proven that bootstrap is a good resampling method for selecting a machine learning model. Bootstrap randomly selects a subset of samples (with replacement) to fit and train the model and the remaining subset to validate the model. An iteration over several times will give a better representation of the samples. After each process, a predictive performance is estimated with the validation set. The average of the scores is considered as the final estimation of the model generalization performance.

2.1.3 Kennard-Stone and SPXY sampling algorithms

Kennard-stone algorithm is probably the best-known method of uniform design among molecular modeling practitioners. The algorithm selects a representative subset according to relatively simple rules that can be summarized in the following steps [1]:

- select object closest to the mean.
- select object that is the most dissimilar to the first
- select object that is the most dissimilar to its nearest object already belongs to the subset
- stop it the subset contains the desired number of objects

The detailed implementation often differs from the general algorithm described previously. There are different measures of dissimilarity, ranging from Euclidean distance to the Tanimoto coefficient that can be used [1]. The DUPLEX algorithm is a modification or extension of the algorithm published by Snee [5]. The algorithm is used to create two subsets (training and test) that have similar statistical properties. Some further often applied subset selection approaches are sphere exclusion [7], OptiMism [3], and D-optimal design [17]. In our study, the Kennard-Stone method is implemented following the description published in [9] with Euclidean distance as a metric. SPXY [6] algorithm is similar to the KS algorithm. The main difference is that SPXY took both X and Y variables into account when calculating the distance between samples. SPXY algorithm used in our study can be found in the work proposed by Wenze Li et al. [11]. The core of KS and SPXY algorithms are maximum-minimum distance split, and we can define another distance metric according to the real situation. Euclidean distance metric was used in this study.

3 Research methodology

The choice of the research methodology is a important steps in a research project. The research method, approach, and strategy used in the study are based on the choice of specific research methodology.

3.1 Choice of research method

A methodology is essential when answering a research question. The choice of a research method depends on the study goal or the expected outcome [13]. A research method can be divided into a qualitative or quantitative group. A qualitative method is used to understand opinion, meaning, and usually performed with small data enough to reach good [13]. On the other hand, A quantitative method formulates objectives that can be evaluate with measurable data. The method is usually performed on large datasets with statistics tools to test the hypothesis [13]. We used a quantitative method in our study for the following reason. First the question of whether data splitting influences or not the machine learning model external predictivity, can be answered by quantifiable metrics. We needed to compare the different splitting algorithms based on the numerical result of our machine learning.

In terms of the research method, the empirical research method was suitable for our work. Conceptual and fundamental research does not fit our study since the goal is not to create new theories or concepts of data splitting algorithms. The applied research method is usually used to solve practical problems. However, the purpose of our study is not to build software or product. So the applied method is not used. The theoretical research method cannot also be used because our goal is not to prove any mathematical theorem or stimulation. Our research's main focus is to study the performance of a machine learning model based on data from a metric (Pearson correlation). The results are inferred from data collections and analysis. Consequently, it is reasonable to adopt the empirical method.

Given that the research will follow the empirical method, the conclusion will be drawn from the research results' quantification. This requires us to find an adequate dataset for the experiments. So the experiment data collection method

fit our study because there are many open data available online for our research purpose. We decided to also use the computational mathematics method in order to simulate data with known errors. After data collection, the next step is the data analysis, and the computational Mathematics method is most appropriate for our case. Our research focuses on machine learning model, which is the main part of computational mathematics [18].

To compare the different splitting algorithms, we will measure the performance of the machine learning model built with the different training sets. So we need a metric that can help us quantify the performance to make an interpretable outcome for our comparison. We are interested to see which data splitting will make the model prediction close to the true values. Pearson correlation is the appropriate evaluation metric, as we wish to see if there is a linear relationship between those variables.

3.2 Application of research method

3.2.1 Data Collection

Simulated data

In this study, simulated data were used to compare the different splitting algorithms. We generated a regression problem base on Friedman one (1) of R package. The algorithm is described by Friedman [1] and Breiman [2]. We simulated different datasets of size,100, 500, and 1000. Friedman algorithm gives ten independent features uniformly distributed on the interval [0, 1]. We also generated data of 1000 samples. This data set is used as a test to evaluate the model performance on unseen data.

Chemoinformatic features of molecules

The real data used in this study is the molecular dataset collected from the dream olfaction challenge website. It consists of 476 structurally diverse odorant molecules. Among the molecules, we can found cyclic molecules, organosulfur molecules, and ester molecules. We generated molecular features with the Dragon software version 6 [34] . Each molecule has 4,884 different chemical

features. In our study, the molecular chemical features were used to predict odor intensity.

The perceptual rating of the odor intensity was originally collected during the smell study[34]. The rating varied between 0 and 100, where 0 means "extremely weak," and 100 is "extremely strong" intensity. Sixty-one people rated the differents molecules without olfaction training. Each molecule was assigned to each subject at high and low concentration. Twenty (20) molecules were tested twice. We have 992 stimuli or data points (476 plus 20 replicated molecules at two different concentrations). The dataset of 476 chemicals was already divided into two subsets 407 for the training set and 69 for the test set. We used the same test set. However, the train set was splitting again into training/validation for building the machine learning model.

3.2.2 Preprocessing of the real data

Data Preprocessing is a technique to clean and prepare data for statistical analysis. For the molecular features, we have removed the columns with constant values or NaN values. After data cleaned, we end up with 3085 features. The molecular input features were also normalized to values between 0 and 1. The formula is given as:

$$x' = \frac{x - min(x)}{max(x) - min(x)}$$ x is the original value and x' the scaled one .

3.3 Generate a random regression problem

Simulated data are widely used to assess optimization methods. This is because of their ability to evaluate certain aspects of the methods under study; these aspects are impossible to look into when using real data sets due to the limited size of data available. The simulated datasets were generated by using the first Friedman function in the R package. It generates a regression problem with samples of 10 dimensions randomly sampled.The algorithm is described by Friedman [1] and Breiman [2]. The function gives two targets Y values, One with noise N(0,1)

and the true values (without noise). This allows us to compute the expected correlation score of the regression problem.

3.4 Software

Python is one of the topmost languages. It is used primarily for performing data analysis. The flexibility and the extended libraries make it more used in a data science project. All the code was written with python 3.6. All the different machine-learning algorithm was built with Sklearn library. Other python libraries, Pandas, Numpy, Scipy, Matplotlib, were used for data manipulation.

3.5 Implementation

Random forest, a popular ensemble learning algorithm for regression and classification [32], was used and applied to simulated and real data. The random forest model has hyper-parameters that need to be optimized. In this study, We have investigated the following four parameters through different splitting algorithms:

- n_estimators: number of trees in the forest. We look for the optimal parameter in the interval [10, 2000].
- max_depth: maximum depth of each tree. We have set an interval of 10 to 110 to search the optimal value. By default, maximum depth is set to None. In this case, each tree of the forest will expand until every leaf is pure.
- max_features: The max_features parameter specifies the size of the random subsets of features to consider when splitting a node.
- ”min_samples_leaf: minimum number of samples needed at a leaf node. By default, we have one (1) sample. The internal range of search was [1-4]” [12].

For each data sampling algorithm (K-fold, Ken-Stone, SPXY, and bootstrap), a parameter is used to divide the data into two subsets: training set and validation set. And we fine-tuned the model to find an optimal random forest model parameters. Below is the list of sampling algorithms and the parameters used in this study:

- Cross-validation: the number of folds was 3, 5, and 10.
- Bootstrap: the number iteration was 10, 50, and 100.
- KS and SPXY: we selected as training set the 10, 20, and also 80% of top-ranked samples.

We tested many parameters to evaluate the effect of data splitting algorithm parameter on model selection. Let consider the case of SPXY algorithm. If the parameter is set to 10%, with a dataset of 100 samples, the training set would only have ten (10) samples, and the validation set 90 samples. We find-tune the

machine learning model with a set of hyperparameters to find the optimal model. Once the optimal model was found, the model is retrained with the full data set. The generalization performance is estimated on the test set. In real-world applications, test sets are usually chosen from the same dataset as the training and validation set. However, in our study, we generated an independent set. The main reason is to have a stable estimation of model performance and avoid the impact of sample size and data splitting methods. Moreover, this is important if we want to have a reliable comparison of the splitting methods and their different parameters. It can only be done when we have access to unlimited samples, such as simulated data.

4 Results

The correlation score of the different data sets is presented in figure 4.1. From the result, it is visible that the most important element is the size of the dataset. The Pearson correlation score (PCS) variations decrease as the number of samples increase. For data of size 1000, the Pearson correlation nearly becomes constant. With a significant representation of samples, there is no important impact of sampling algorithm on the model generalization performance. However, on small datasets (100 samples), there was a significant variation of the validation set PCSs. This shows how it is important to have a good data sampling strategy when working with a small dataset to get the best possible model.

We noticed a significant variation within the Pearson correlation scores (PCSs) on the validation set than those for the test set, particularly with a small dataset of 100 samples. Overall, the models overfitted, the PCSs of validation sets were above those of blind sets; this is consistent with previous researches [2]. The KS algorithm showed the most significant variations in PCSs of validation sets. When a small set of samples was used as a training, the estimated correlation of the validation set was lower than the test set. However, The model overfitted when much data (>60%) were selected. The estimated correlation of the test set was lower than the validation set.

When comparing the result of the models built based on KS and SPXY on both simulated and real data, SPXY generated more over-optimistic estimations than K-S. On simulated data of size 100, SPXY reached a correlation of 85% on the validation set, when only 40% of the samples were used for training. However, K-S needed at least 60% of samples to achieve the same PCSs. When 40–60% samples were used to train the model, the gap between the validation and test sets was much smaller in terms of the PCSs. The difference between these two types of PCSs was still much more significant than k-fold cross-validation splitting. It is important to acknowledge that there are other sampling algorithms [28–30], which may perform better.

When the model was trained based on the K-fold splitting, we observed a few variations in term PCSs for validation sets. Furthermore, the variations were

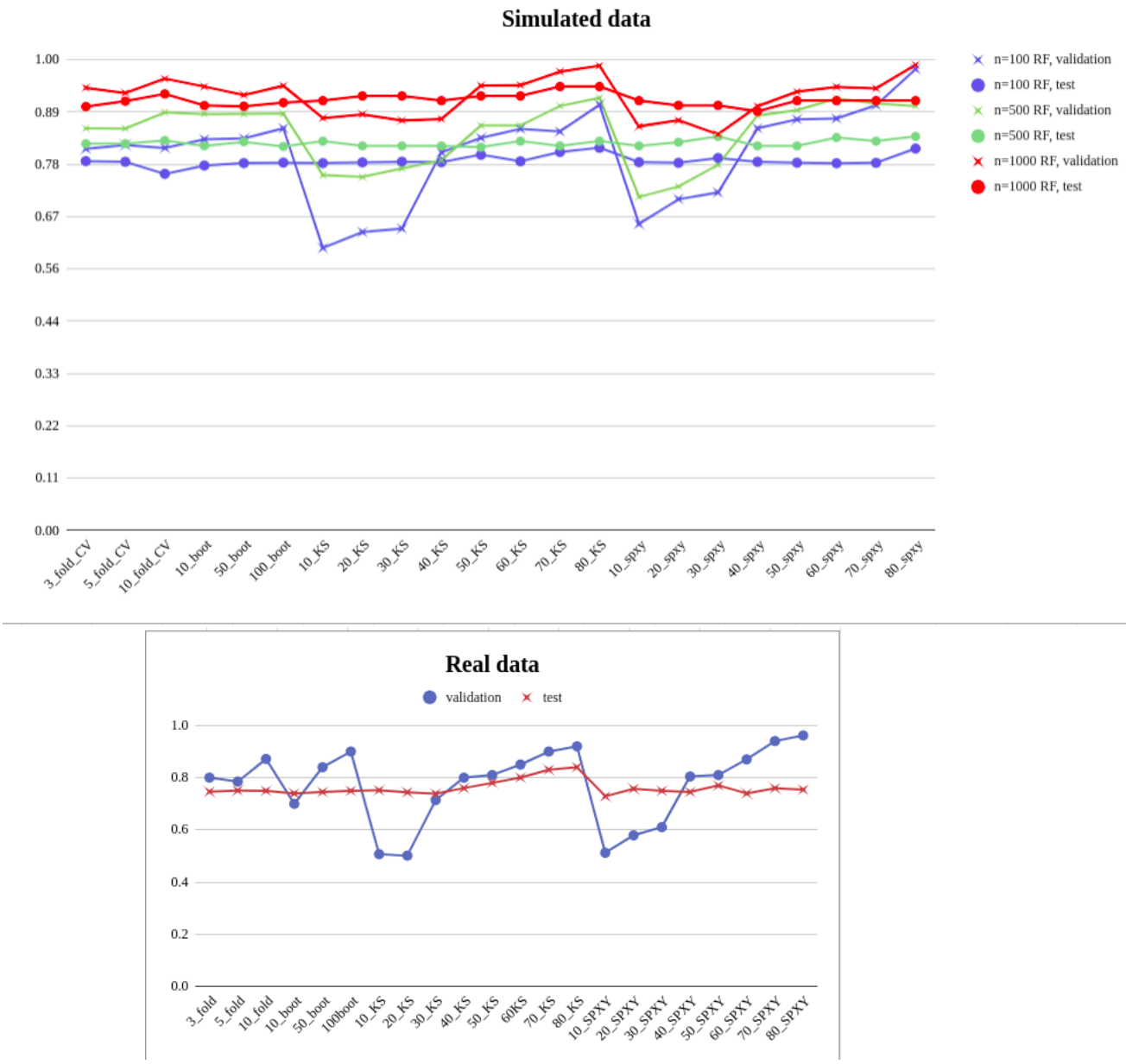

Figure 4.1: Pearson correlation scores for both simulated and real data.

still relatively low than the PCSs of the test sets. When the training data was very small or too many, the difference in terms of Pearson correlation between the validation and test set was more significant with the k-fold algorithm. This highlighted the importance of having a balanced training and validation set size for good model generalization and to avoid overfitting. When implementing a machine learning model, one may think that adding more samples in the training set will improve the model's performance. However, in real-world applications, there is no other data available excepted the external test set. This can make the external test set smaller and result in a worse scenario with a bad generalization performance.

5 Analysis

In this study, we carried comparative analyses of data splitting algorithms for machine learning model selection. The outcomes of our research suggested that most sampling algorithms with typical parameters can have the same result; So, they are all good for model selection. Still, the high variation of the correlation score on the validation shows that the model was sensitive to the sampling algorithms, mainly with small samples of size 100.

The Pearson correlation scores of the models build based on the splitting algorithms are presented in Figure 4.1. From the result, no sampling algorithm is better than others the optimal model parameters finding. Indeed, the estimated correlation score on the test set was approximately the same for most sampling algorithms. However, when considering the difference between the validation and test score, some splitting algorithms were better. Even with the large interval of parameter settings used for every sampling algorithm, finding a splitting method, which was significantly better than the other methods, was rare. It was challenging to choose which combinations of methods and parameters were the most suitable for selecting a machine learning model. An overall impression is that with a random splitting algorithm, and a reasonable selection of the training/validation set, we can still achieve the same result as k-fold or rational splitting algorithms.

The Friedman one algorithm helped generate a regression problem with two targets output one with Gaussian noise and one with the true target value(without noise). The correlation between the two targets gives an idea of an expected score. This allowed us to evaluate the estimated generalization score with the expected one. However, the best optimal model did not reach 98% (the expected correlation score). In general, we found that PCS was higher when there was more data.

6 Concluding remarks

6.1 Conclusions

In this study, we found that model performance improved when there was more data. The answer to the question of how the choice of data splitting algorithm can improve the estimation of the generalization performance is data dependent. When the size of the data is big, the data splitting algorithms do not influence the result. However, when small data was used, data splitting algorithms can improve generalization performance. This resulted in the conclusion that there is no definite proof suggesting which method and parameter combination would always provide significantly better results than others. The chosen method for data splitting and which parameters to use cannot be decided a priori and would be data-dependent. However, a good balance between the size of the training, validation, and test set can give a stable estimation of model performance.

6.2 Validity and Reliability

We have followed the best practice for machine-learning project development to ensure the validity and the reliability of our solution. Indeed, for each splitting algorithm, we implemented specific machine learning model. Evaluating with one single model would have lead to another problem,the choice of parameter such as the number of tree for the random forest. So We selected the best model hyper-parameters specific to the splitting algorithm to avoid the influence of other data partitioning algorithms such as cross validation. In order to minimize the error in our code, we have used the algorithm and function from python libraries. However, the results shown are by no means exhaustive,there are other data splitting methods [24-26] may give better result.

6.3 Reproducibility

The code and dataset for rational splitting are available for use on the github. The Java software can be found here: http://sci2s.ugr.es/sicidm

6.4 Future work

Our suggestion for future work is to generate another type of data with different distributions; and evaluate the different algorithms with deep learning model to see if we can draw the same conclusion.

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