ABSTRACT

In machine learning, a routine practice is to split the data into a training and a test data set. A proposed model is built based on the training data, and then the performance of the model is assessed using test data. Usually, the data is split randomly into a training and a test set on an ad hoc basis. This approach, pivoted on random splitting, works well but more often than not, it fails to gauge the generalizing capability of the model with respect to perturbations in the input of training and test data. Experimentally, this sensitive aspect of randomness in the input data is realized when a new iteration of a fixed pipeline, from model building to training and testing, is executed, and an overly optimistic performance estimate is reported. Since the consistency in a model’s performance predominantly depends on the data splitting, any conclusions on the robustness of the model are unreliable in such a scenario. We propose a diagnostic approach to quantitatively assess the quality of a given split in terms of its true randomness, and provide a basis for inferring model insensitivity towards the input data. We associate model robustness with random splitting using a self-defined data-driven distance metric based on the Mahalanobis squared distance between a train set and its corresponding test set. The probability distribution of the distance metric is simulated using Monte Carlo simulations, and a threshold is calculated from one-sided hypothesis testing. We motivate and
While much of the existing works have been dedicated to finding an ideal data split for model building and evaluation, what type of model will be used on them. A proposed Monte-Carlo simulation-based hypothesis test checks the performance of the existing data splitting methods using the proposed method.}

Keywords Random splitting · Mahalanobis squared distance · Train-Test Split · Diagnostics · Distance Metric

1 Introduction

Statistical or machine learning models are used for inference and prediction. The purpose of inference is to understand or test hypotheses about how a system behaves, whereas prediction aims to forecast unobserved outcomes or future behavior (Bzdok et al., 2018). When the sole objective is to infer the association (or causality), people do not split the data into training and test sets. For example, in a randomized controlled trial (RCT), researchers use the entire data to find out whether a treatment is more effective than the other treatment or placebo (Friedman et al., 2015). On the other hand, it is common in supervised machine learning tasks, where the goal is prediction, to split the data into training and test sets for model development and evaluation, respectively (Hastie et al., 2009; Stone, 1974). The model is fitted using the training data by estimating parameters and functions. Afterward, the developed model is assessed using the test data.

Birba (2020) provides a comprehensive comparison of various data splitting methods employed in machine learning. This work also demonstrates how different data splitting strategies affect the estimation of the generalizing ability of a model. They experiment with techniques like k-fold cross validation (Kohavi et al., 1995), bootstrap-based random splitting, Kennard and Stone (K-S) algorithm (Kennard and Stone, 1969), and SPXY algorithm (Galvão et al., 2005). They conclude that data splitting is a heuristic step and its relation to model performance is dependent on the underlying data. A widely accepted notion for obtaining reliable model performance is that the underlying training and test sets agreeably represent the entire dataset. The K-S algorithm and its successor SPXY algorithm are built on the stated notion and aim to preserve original data information in the selected subsets. Naturally, the CADEX (K-S algorithm) and SPXY algorithms depend on an underlying distance metric, often chosen as the Euclidean distance. The fundamental difference between them is that SPXY considers the statistical variation of the dependent variable along with independent variables while choosing the best representative subset, while CADEX only considers independent variables. Galvão et al. (2005) argue that this inclusion leads to a more effective distribution of data samples in the multidimensional space and thus enhances the model’s predictive ability. Joseph and Vakayil (2021) develop a new data splitting method (SPit) based on support points and compare their strategy with the deterministic CADEX (K-S algorithm) and DUPLEX algorithms in their work. The SPit method follows a similar ideology while segregating samples into training and test sets. They choose the most representative data points for testing and use the remaining for training. They find optimal representative points or Support Points (SP) of the entire dataset and then employ nearest neighbors technique to sequentially subsample from the dataset. On comparing their method with the existing CADEX and DUPLEX subsampling techniques, they reported substantial improvement in the worst-case predictions. Choosing a test set that mimics the entire dataset is not the best policy for concluding model robustness, as even a bad model can perform well on an engineered split. Xu and Goodacre (2013) found that K-S and SPXY had poor performance estimates of model performance since the most representative samples are chosen first, leaving a poorly representative sample set for model performance estimation.

The existing splitting methods aim to divide the data sets into training and test sets with the same distribution as the original data. Let us call it an ideal data split. Do we need that kind of split? In practice or production, the model performance will be assessed through new data that is expected to differ from the existing data. Ideally, we may want to test a developed model using a dataset having the same distribution as the training data and using another dataset whose distribution deviates (reasonably) from the training data. A good performance with the former type of data ensures that the model works well when the new data has the same distribution as the training data. Further, a poor performance indicates that the model is unsuitable for deployment or solving the task at hand and may be discarded. On the contrary, we do not expect good performance in the second testing environment. However, if we observe a reasonable performance with data whose distribution deviates from the training set distribution, it indicates the developed model’s robustness to perturbations in new data.

While much of the existing works have been dedicated to finding an ideal data split for model building and evaluation, analyzing the quality of a particular data split has not been discussed extensively in the literature due to the heuristic nature of data splitting methods. In this light, this paper presents a new perspective on data splitting. We propose a diagnostic approach method pivoted on the formulation of a new distance metric based on the Mahalanobis squared distance (McLachlan, 1999) followed by a hypothesis test to assess the quality of a data split (random or non-random). The Mahalanobis squared distance-based proposed metric calculates the multivariate distance between the training and test data sets. The advantage of the proposed method is that it assesses the quality of a data split without considering what type of model will be used on them. A proposed Monte-Carlo simulation-based hypothesis test checks the similarity of the distribution in the training and test data sets. In addition to that, if the model (say a regression model)
is decided, then we also show (in the graph) the relative performance of the model on the given split with respect to all possible splits using the normalized Akaike Information Criterion (AIC) [Sakamoto et al., 1986].

The paper is organized as follows. Section 2 describes different splitting strategies with examples. Section 3 discusses the methodology underlying the proposed method. It formulates the hypotheses and describes the algorithm. The results of various experiments using real data are given in Section 4 along with a discussion of critical observations. Section 5 presents the conclusions regarding the method and its applicability.

2 Different Splittings Strategies and Examples

The simplest and perhaps most common strategy to split a dataset and obtain the corresponding training set (and test set) is to sample a fraction (say 80%) of the dataset randomly. This strategy is referred to as random splitting. Other techniques like cluster-based splitting, stratified splitting, and adversarial or biased splitting [Søgaard et al., 2020] can be used and are examined in Figure 1. The underlying data is a hypothetical dataset of sports players and their net worth. We assume an objective of associating a player’s net worth with the sport they play and compare the four data splitting strategies by plotting Sport vs. Net Worth. It is expected that different splitting techniques will produce different train-test partitions for a given split percentage. Stratified splitting or stratified random sampling obtains a sample population that best represents the entire population under investigation. Consequently, in Figure 1a, approximately 60% entries from each sport are randomly chosen for training while the remaining are kept for testing purposes. Class imbalance achieved after partitioning the data sorted on net worth, as shown in Figure 1b, is a classic example of introducing an adversarial effect. Adversarial splits are a great way to examine the true capability of a model. Søgaard et al. [2020] conclude that multiple biased splits give a more realistic estimation of out-of-sample error as compared to multiple random splits. Another typical technique to split a dataset is cluster-based splitting. In Figure 1c, the complete dataset is split by forming clusters of sports. Considering a split percentage of 50%, we randomly assign 2 clusters to the training set and the remaining 2 clusters to the test set. Finally, Figure 1d portrays random splitting where no restrictions are in place. All data points are pooled together and split into two subsets comprising 60% (training) and 40% (test) of the data, respectively. In particular, a random split with 60% split percentage can result in the following outcomes:

1. More than 60% entries from a sport in the training set (Basketball).
2. Less than 60% entries from a sport in the training set (Football).
3. Exactly 60% entries from a sport in the training set (Cricket).

Figure 1: Data splitting strategies. Each subplot represents a splitting technique. Each ball in a subplot corresponds to a player. Blue (dark) / orange (bright) balls represent examples for test / training. The split percentage is considered to be 60% for stratified splitting, adversarial splitting, and random splitting. A split percentage of 50% is considered for cluster-based splitting.
Accordingly, Figure 1 shows how random splitting differs from other techniques and highlights its indifferent behavior towards maintaining similar distributions of the training and test sets. Generally, the randomness induced by the random splitting method eliminates subtle biases that might impede a conclusive evaluation of the model.

Apparently, the random split should maintain the same statistical distribution of the original data in the training and test data. However, in practice, we may see the distributions in the training and test vary a lot after random splitting. Figure 2 presents two scenarios of random splitting of the original data. To illustrate how random splitting can highly influence the model assessment, we fit a regression model into the training data and assess its performance in the test data. We consider \( R^2 \) values to assess the model performance. Note that \( R^2 \) value for the test set is not the conventional \( R^2 \) value. It is calculated using the predicted value of weight (response) using the regression model fitted in the training data. Figure 2 uses the Abalone Dataset from the UCI Machine Learning Repository to regress the weights of 4177 abalone fishes with their heights. In the first scenario, the first row of Figure 2 the test \( R^2 \) is much higher than the training \( R^2 \), indicating a good model fit. In the second row, the test \( R^2 \) drops compared to the corresponding training \( R^2 \). The drop in the model performance is a consequence of the position of two apparent outliers (Osborne and Overbay, 2004), without going into further detail to decide whether they are influential or outlier points. In summary, we observe that when both the outliers are in the training set (Figure 2a), the corresponding test set reports a higher \( R^2 \) (Figure 2b). In contrast, the presence of an outlier in the test set (Figure 2d) and the other in the training set results in a drop in the \( R^2 \) value. This example shows that two simulations yield significantly different model performances for the same model relation. Since the behavior is ambiguous and depends on the underlying data split that led to the variation, it is difficult to estimate the correct model performance.

Another example, shown in Figure 3, portrays a similar ambiguous behavior in estimating model performance. The dataset used in Figure 2 is the Diamonds dataset with 53,940 entries available in the ggplot library in R. We attempt to map out the price of the diamond based on the carat of the diamond used. We use a polynomial regression model and the normalized AIC score as discussed in Section 3.4. A drop (higher AIC) in the test model performance signifies that random splitting can lead to ambiguous model performances. Consider the first simulation for this dataset in Figure 3a where the split percentage is 80%. We observe a strong model performance on the test split and the train split conclusive of a robust model. Although, in the second simulation, the normalized AIC score goes to 16.916 due to an adversarial data split, indicating a poor model performance on the test split when compared with the corresponding train split as well as the previous simulation.

Therefore, different random splits can lead to different model performances, making any conclusions about model robustness unreliable. To tackle this selection bias or prevent overfitting, researchers have employed other model evaluation techniques like cross-validation (Refaelzadeh et al., 2009) which provide efficient estimates by averaging the model performance over a number of train-test splits. Although, this method is computationally expensive and often infeasible on large datasets due to repeated training of the model.

Thus, it raises the need for a method to correctly estimate the model performance without re-training the model or even knowing the model relation. Since the variation in model performance is primarily precipitated by the random splitting step, we propose a statistical technique to diagnose and classify splits as "good" or "bad". A good split would yield reliable model performances, while a bad split will not. Before we proceed to the method, we discuss Mahalanobis squared distance in the next section.

3 Methodology

3.1 Mahalanobis Squared Distance

Distance measures are essential components of numerous machine learning techniques (Xiang et al., 2008). Classification algorithms like KMeans (Krishna and Murty, 1999) and K-nearest neighbor (KNN) (Peterson, 2009) are supported by such metrics due to their need of a suitable distance metric for identifying neighboring points. One such widely used distance measure is the Mahalanobis squared distance (McLachlan, 1999). The Mahalanobis squared distance is the distance of an observation \( x \) from a set of observations with mean vector \( \mu \), and a non-singular pooled covariance matrix \( \Sigma \). It is expressed as

\[
\Delta^2 = (x - \mu)^T \Sigma^{-1} (x - \mu). \tag{1}
\]

The use of Mahalanobis squared distance has grown over the years. It is used in data clustering, image segmentation, and face pose estimation problems (Xiang et al., 2008). A modified version of the distance is used in classification tasks executed through K-nearest neighbors in a multivariate setup (Galeano et al., 2015). The Mahalanobis squared distance takes into account correlations and scales of variables (Brereton and Lloyd, 2016) and it is also used for outlier detection (Geun Kim, 2000).

1When comparing two models, the one with the lower normalized AIC score is considered to be a more robust model.
A Diagnostic Approach to Assess the Quality of Data Splitting in Machine Learning

Figure 2: **Drop in model performance:** The objective is to regress the weight of the species with their height. The data is represented using blue dots. The orange line represents the linear regression model fitted on train set.

The basic notion for obtaining a good train-test split is to make the distribution of the training set and the test set close to each other. In other words, the farther the test distribution from the training distribution, the less accurate estimate of model generalizability is reported. Building on this notion, we try to find the distance between the training and the test sets. Inspired by the pervasive use of the Mahalanobis squared distance, initially proposed by [Mahalanobis (1936)] in statistical as well as machine learning tasks, we define a new distance metric based on it. We use it to quantify the distance between any two population samples, more particularly, training and test samples. We use this distance metric to ultimately diagnose the quality of a random split irrespective of the model relation and the problem type through Monte Carlo simulation-based hypothesis testing [Theiler and Prichard (1996)] discussed in the next section.

### 3.2 Distance Metric

As discussed in Section 3.1, we use the Mahalanobis squared distance to calculate the distance between two multivariate populations. Consider $\mathbf{X} = (x_1, x_2, \ldots, x_{n_X})^T$ and $\mathbf{Y} = (y_1, y_2, \ldots, y_{n_Y})^T$ to be the two data samples with $n_{X}$ and $n_{Y}$ be the number of observations, respectively. Let $\mu_X$ and $\mu_Y$ be the means of the two corresponding populations. Further, obtain the pooled variance-covariance matrix $\Sigma_p$ of entire data as,

$$
\Sigma_p = \frac{(n_X - 1)\Sigma_X + (n_Y - 1)\Sigma_Y}{n_X + n_Y - 2}
$$

(2)
A Diagnostic Approach to Assess the Quality of Data Splitting in Machine Learning

Figure 3: **Drop in model performance**: The objective is to associate the price of the diamonds with the carats of the diamond. The data is represented using blue dots. The orange curve represents the polynomial regression model fitted on train set.

From (1), we calculate the distance of each observation \( x_i \) from the other population \( Y \) using (3). Similarly, we calculate the distance of each observation \( y_j \) from the population \( X \) using (4). The two distances are given as:

\[
\Delta^2_{x_i Y} = (x_i - \mu_Y)^T \Sigma_p^{-1} (x_i - \mu_Y), \quad \forall i = 1 \ldots n_X, \tag{3}
\]
\[
\Delta^2_{y_j X} = (y_j - \mu_X)^T \Sigma_p^{-1} (y_j - \mu_X), \quad \forall j = 1 \ldots n_Y, \tag{4}
\]

respectively. We assume that the training and the test data sets have the same variance-covariance structure and it can be represented by (2). The two expressions in (3) and (4) calculate the distance of a single observation of \( X \) from \( Y \) and of \( Y \) from \( X \), respectively. Further, we define the average distance of population \( X \) from population \( Y \), and vice-versa as,

\[
\Delta^2_{XY} = \frac{1}{n_X} \sum_{i=1}^{n_X} (x_i - \mu_Y)^T \Sigma_p^{-1} (x_i - \mu_Y), \tag{5}
\]
\[
\Delta^2_{YX} = \frac{1}{n_Y} \sum_{j=1}^{n_Y} (y_j - \mu_X)^T \Sigma_p^{-1} (y_j - \mu_X), \tag{6}
\]

respectively. Finally, we calculate our distance metric \( \Lambda \) as the average of the newly defined distances, \( \Delta^2_{XY} \) and \( \Delta^2_{YX} \) as,

\[
\Lambda = \frac{\Delta^2_{XY} + \Delta^2_{YX}}{2}. \tag{7}
\]

We denote the two populations \( X \) and \( Y \) to be the training set and the test set, respectively. After quantifying the distance between the training set and the test set, the question remains whether a small distance between these samples
A Diagnostic Approach to Assess the Quality of Data Splitting in Machine Learning

is conclusive of a good train-test split, and if so, can we infer model robustness using it? To answer this question, we devise a hypothesis test which checks whether the training set and the test set follow a similar distribution or not. In the next subsection, we formalize our strategy for hypothesis testing and provide a Monte Carlo simulation-based algorithm to implement the same.

### 3.3 Monte Carlo Method for Hypothesis Testing

Intuitively, we formulate our null hypothesis that the training data and the test data corresponding to a good train-test split follow a similar distribution. The implicit assumption here is that when two populations are sampled from a common underlying distribution, the distance between the two populations is arbitrarily small. We use (7) to calculate the distance between the two sets. The hypotheses can be formalized as follows.

- **$H_0$**: The training data and the test data corresponding to the train-test split follow a similar distribution.
- **$H_1$**: The training data and the test data corresponding to the train-test split don’t follow a similar distribution.

We perform a one-sided $\alpha$-level hypothesis test (Ruxton and Neuhäuser, 2010) for our setup and calculate the value of the test statistic $\Lambda$ as $\Lambda_{\text{obs}}$, the distance metric for the given split, using (7). To simulate the probability distribution of $\Lambda$, we run multiple simulations, i.e., repeatedly split the dataset into training and test, and calculate the distance metric for each simulation. Note that $\Lambda$ takes only positive values. Reusing the same notation, let $\Lambda$ be the random variable having the above simulated distribution. Further, we reject the null hypothesis when $\Lambda$ is greater than some constant $c > 0$. Consequently, for a given $\alpha$, we calculate the $c$ using

$$P_{H_0}(\Lambda > c) \leq \alpha. \quad (8)$$

Based on the rejection criterion, we will judge the quality of the random split and classify it as a good train-test split for model evaluation. We also find the $p$-value as follows,

$$p = P_{H_0}(\Lambda > \Lambda_{\text{obs}}). \quad (9)$$

Figure 4 describes the major steps of the entire process. It explains the procedure as a combination of three major steps. The first step is to calculate the test statistic $\Lambda_{\text{obs}}$ using (7) for the input partition. Next, we obtain the complete dataset by joining the training partition and the test partition. Once we have the entire dataset, we repeatedly split (with the same split-percentage) the dataset under the random splitting paradigm and calculate the distance value for each of the random splits. After $N$ simulations, we obtain a vector of distance values for a given dataset. If $N$ is large enough, we can assume that this vector simulates the probability distribution of the test statistic $\Lambda$. Finally we reject the null hypothesis if $\Lambda_{\text{obs}} > c$. Algorithm 1 describes the entire process.

**Algorithm 1 Monte Carlo Simulation based Hypothesis Test**

**Require**: $X$, $Y$, $\alpha$, $N$

1. $\Lambda_{\text{obs}} = \text{calculate\_distance}(X, Y)$
2. Initialize $D[1, \ldots, N]$ to store the distance metric values
3. Join $X$ and $Y$ sets to obtain the entire dataset ($df$)
4. $s = \text{calculate\_split\_percentage}(X, Y)$
5. for $j = 1$ to $N$ do
6. $(X, Y) = \text{random\_split}(df, s)$
7. $\Lambda = \text{calculate\_distance}(X, Y)$
8. $D[j] = \Lambda$
9. end for
10. $p = \text{calculate\_pvalue}(D, \Lambda_{\text{obs}})$
11. if $p > \alpha$ then
12. Accept Null Hypothesis
13. else
14. Reject Null Hypothesis
15. end if

### 3.4 Association of model performance with distance metric

Generally, there are several attributes (or features) in real-life datasets. Choosing a subset of these attributes to establish a definite model relation a priori is unexpected and uncommon. In this light, we presented the above
A Diagnostic Approach to Assess the Quality of Data Splitting in Machine Learning

Figure 4: Monte Carlo simulation-based hypothesis testing procedure.

technique, which works on the entire dataset without assuming any learning objective or model relation or fitting any regression/classification models. However, if the model relation is provided, the proposed method can associate model performance with the defined distance metric through a simulation plot.

The Akaike Information Criterion ([Burnham and Anderson] [1998] [Sakamoto et al.] [1986]) is used as the performance metric as,

\[ AIC = -2 \log(\mathcal{L}(\hat{\theta}|x)) + 2K \] (10)

where \( \mathcal{L} \) is the maximum value of the likelihood function for the model, and \( K \) is the number of parameters in the model. In ordinary least squares regression, the residual sum of squares (RSS) ([Draper and Smith] [1998]) is calculated as,

\[ RSS = \sum_{i=1}^{n}(y_i - \hat{y}_i)^2 \] (11)

where \( y_i \) is the \( i^{th} \) observed value of the response variable, and \( \hat{y}_i \) is the \( i^{th} \) predicted value of the response variable. Thus, in case of ordinary least squares regression ([Burnham et al.] [2011]),

\[ \log(\mathcal{L}) = -\left(\frac{n}{2}\right) \log \left( \frac{RSS}{n} \right), \] (12)

which gives

\[ AIC = n \log \left( \frac{RSS}{n} \right) + 2K. \] (13)

Since AIC is dependent on the sample size \( n \), we will use the normalized form of the metric to make it invariant to sample size ([Cohen and Berchenko] [2021]). The normalized AIC is obtained by dividing the AIC score by the sample size and can be expressed as,
A Diagnostic Approach to Assess the Quality of Data Splitting in Machine Learning

\[ AIC_N = \log \left( \frac{RSS}{n} \right) + \frac{2K}{n}. \]  
(14)

For visualizing different simulations (data splits), we repeatedly split the dataset, train the model using the given model information, calculate the distance metric between the training and test sets, and measure the model performances for both sets using (14).

In the next section, we provide examples through real-life regression datasets when the model information is provided and when it is not. We discuss the output plots and potential conclusions drawn from them.

4 Experiments and Results

We consider regression analysis to present the findings computationally. The datasets used for the experiment are discussed below. For all the datasets, we run Algorithm (1) and obtain a conclusion regarding the quality of the random split using R.

Abalone: This dataset is taken from the UCI Machine Learning Repository (Dua and Graff, 2017). This data came from an original study conducted by WJ Nash (Nash, 1994). There are 9 variables, out of which one is an ordered factor, one is an integer, and the rest are continuous variables. The predominant purpose of the dataset is to predict the age of abalone, characterized by the variable Rings, from their physical measurements. We consider a regression model with Rings as the response variable and independent variables as LongestShell, Diameter, and Height. Here, LongestShell denotes the maximum length of the shell of abalone, the Diameter is the length perpendicular to the longest shell, and Height is the height of abalone. The information has been tabulated in Table 1.

| Attribute                        | Abalone dataset | Diamonds dataset |
|----------------------------------|-----------------|------------------|
| No. of Rows (Sample Size)        | 4,177           | 53,940           |
| No. of Columns (Variables)       | 9               | 10               |
| Model Relation (Regression)      | Rings ~ LongestShell + Diameter + Height | price ~ volume + depth |

Diamonds: It is available in the ggplot2 library in R. There are a total of 10 variables, out of which three are ordered factors, one is an integer, and the remaining six are numeric. These variables measure the various characteristics of 53940 round-cut diamonds. We define the regression model with price as the response variable and independent variables as depth, x:y:z. Here, price denotes the price of the diamond in US dollars, depth denotes the total depth percentage, and x, y, and z denote the length, width, and height in millimeters respectively. The product, x:y:z, of the three dimensions x, y, and z can be interpreted as the volume of the diamond. The above relation precisely conveys that the price of the diamond is a linear combination of the depth percentage of the diamond and its volume. The information has been tabulated in Table 1.

4.1 Models and Metrics

We present four examples, two for each dataset. Figure 5a shows a random split with seed as 3. Using Algorithm (1) and comparing the given split with approximately all possible splits, the proposed method accepts the null hypothesis to conclude that the training set distribution and the test set distribution are similar. Accepting the null hypothesis indicates that model performance measured corresponding to the generated split is reliable. Figure 5b shows another simulation for the abalone dataset with seed as 20. We observe that the null hypothesis is rejected as the split lies in the right-most clusters in the simulation plot of Figure 5b. According to our analysis, this split is not a good split to assess model performance as it is a corner case, and a poor model performance on such a split doesn’t signify a poor model. Although, a good model performance on such a split can ensure model robustness. Table 2 summarizes the two simulations.

A similar experimental analysis for the Diamonds dataset is held. A random split with seed 2 results in the null hypothesis being accepted. The simulation is visualized if Figure 6a. The random split lies in the left region of the simulation plot of Figure 6a indicating a small distance between the training set and the test set. We conclude that this split can be used for measuring model performance. On the other hand, a random split with seed 1 ends up being rejected since the distance between the training set and the test set is large. This split is not ideal for measuring model performance since it is a corner case and can potentially underestimate model performances even for a good model. The results for the two simulations have been collected in Table 2.
A Diagnostic Approach to Assess the Quality of Data Splitting in Machine Learning

Figure 5: Simulations for Abalone Dataset. We regress the Rings of abalone using the longest shell, diameter and the height of the abalone.

Table 2: Conclusion table for simulations on both datasets.

| Attribute                              | Abalone dataset          | Diamonds dataset        |
|----------------------------------------|--------------------------|-------------------------|
|                                        | Run 1 | Run 2 | Run 1 | Run 2 |
| R seed                                 | 3     | 20    | 2     | 1     |
| Distance Metric (Å)                    | 3.912 | 4.825 | 2.911 | 3.331 |
| Limiting Threshold (c)                 | 4.768 | 4.772 | 3.324 | 3.319 |
| p-value                                | 0.27  | 0.005 | 0.845 | 0.025 |
| Model Performance for Initial Train Split | 1.868| 1.835 | 14.941| 14.707|
| Model Performance for Initial Test Split | 2.056| 2.305 | 14.704| 15.444|
| Split Conclusion                       | Accepted | Rejected | Accepted | Rejected |
A Diagnostic Approach to Assess the Quality of Data Splitting in Machine Learning

![Simulation Plot](image1)

![Hypothesis Testing Plot](image2)

(a) Diamonds Dataset for seed = 2 (null hypothesis accepted).

(b) Diamonds Dataset for seed = 1 (null hypothesis rejected).

Figure 6: Simulations for Diamonds Dataset. The price of the diamond is regressed using the volume $(x:y:z)$ and the depth of the diamond.

4.2 Comparison of Existing Data Splitting Methods

We also compare existing data splitting strategies like SPlit (Joseph and Vakayil [2021]), CADEX (Kennard and Stone [1969]), and DUPLEX (Snee [1977]) on the Abalone dataset. We compare the splits produced by these methods among the other possible splits. We visualize the presence of the initial split and conclude their appropriateness based on the hypothesis testing method discussed in Section 3.3. In comparing, we observe that splits produced by the CADEX (Figure 7a), and DUPLEX (Figure 7b) subsampling methods are rejected by our hypothesis testing method. This points out that the split obtained through these methods is not ideal for measuring model performance. On the other hand, the SPlit method developed by Joseph and Vakayil (2021), does produce an acceptable split (Figure 7c). Although concluding model robustness from SPlit’s split is not recommended, it may overestimate the model performance owing to the equitable representation of entire data in the test set.

4.3 R-Package

An R-package is developed to implement the proposed methodology easily for users. The same is available from [https://github.com/eklayaj/RRandomSplitDiagnostics](https://github.com/eklayaj/RRandomSplitDiagnostics)
A Diagnostic Approach to Assess the Quality of Data Splitting in Machine Learning

Figure 7: Comparing different splitting techniques using our hypothesis testing method.


5 Conclusions

Random splitting is the most common method used for data splitting in machine learning tasks. The proposed method includes a data-driven distance metric based on the Mahalanobis squared distance. We simulate the distribution of the distance metric by repeatedly splitting the data in a random manner and calculating the corresponding distance metric. We then impose an $\alpha$-level one-sided hypothesis test with the null hypothesis stating that the training set and the test set of a train-test split follow a similar distribution. The proposed method diagnoses a given split among all possible splits for that dataset. Further, we compare various existing data splitting techniques using the proposed method and discuss whether splits produced by them as good or not for measuring reliable model performance. The ability of our method to gauge the "goodness" of any given split among all other possible splits is one of a kind. We provide a diagnostic approach to assess the quality of a suitable split based on the type of problem at hand. Our method can also be used to judge train-validation splits by changing the initial split input to the algorithm. There is the scope of research to extend the proposed method to consider ordinal and nominal variables by using a generalized form of Mahalanobis squared distance as done by De Leon and Carriere (2005).

We have applied our method to several regression datasets using different choices of model relations and found that it accurately diagnoses the input splits. The use of Monte Carlo simulations in the hypothesis test allows the method invariant to the dataset. Due to its dynamic nature, the proposed method is valid not only for random splits but also for any given adversarial split. Finally, the proposed method assesses the quality of a train-test data split without considering any model relation. However, if the model is specified, it can also compare the relative performances of the model in training and test data concerning all possible splits.

Acknowledgments

J. Neeraja would like to acknowledge the Samsung Fellowship for this work. Palash Ghosh would like to acknowledge support by the ICMR Centre for Excellence, Grant no. 5/3/8/20/2019-ITR.

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A Diagnostic Approach to Assess the Quality of Data Splitting in Machine Learning

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