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# COMMON PITFALLS IN EVALUATING MODEL PERFORMANCE AND STRATEGIES FOR AVOIDANCE IN AGRICULTURAL STUDIES

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## ABSTRACT

This study critically examines the methodologies and metrics used for evaluating prediction models in regression and classification tasks, making a case for the application of rigorous and standardized approaches in model performance assessment. Within the context of this work, we define modeling as a structured framework for hypothesis formulation and decision-making, which relies on the analysis and extrapolation of empirical data. The advancement of modeling is contingent on the accumulation of prior knowledge within the scientific community. The study conducted a series of simulations to delve into common pitfalls in cross-validation (CV), a technique crucial for characterizing expected model performance on “new” data. Issues such as using the same data for both training and assessment, excluding model selection from CV, and overlooking experimental block effects were explored through simulation examples. Moreover, the simulations in this study highlight that no single model performance metric suffices to represent model performance adequately and conservatively, emphasizing the need for understanding the underlying theory of each metric to avoid misleading conclusions. In conclusion, this simulation study aims to guide researchers in accurately and consistently reporting model performance, thereby supporting integrity and scientific rigor in prediction modeling research.

**Keywords** Model Evaluation · Performance Metrics · Simulation Studies

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17 **1 Introduction**

18 **1.1 Review on ultrasound imaging technology**

19 **1.2 Modeling**

20 Modeling is an essential tool for hypothesis formulation and decision-making. It functions as a structured investigatory  
21 framework that allows researchers to explore system understanding through the summary and analysis of empirical data.  
22 Carefully constructed and evaluated models offer the potential to extend this understanding by enabling the extrapolation  
23 of results to novel trials and conditions. Although only one focus of the science of modeling, the predictive role is  
24 often explicitly or implicitly the ultimate goal of models derived within the precision agriculture context. Through  
25 this lens, modeling provides opportunity to standardize and formalize research advancement, through developing  
26 quantitative constructs that accumulate prior knowledge derived by the broader the scientific community. Evaluating  
27 model performance becomes particularly critical when considering this role within the knowledge generation enterprise,  
28 necessitating a rigorous and standardized approach that allows for both reproducibility and comparability. As more and  
29 more model-based exercises are developed using slightly different methods, or slightly different datasets, it becomes  
30 increasingly challenging to evaluate, characterize, compare, and balance information generated by the resulting modeling  
31 tools, particularly when results are conflicting. Specifically, reporting model performance through poorly-defined  
32 metrics or incomplete procedures can create opportunity for confusion, misinterpretation, and miscommunication, and  
33 can ultimately result in distrust in model-based tools and impede scientific progress.

34 Here, we review two types of challenges that can be encountered during the model evaluation process: challenges in  
35 data structure and challenges in evaluation approach. Data structure challenges include those inherent to the types  
36 of data used in a modeling exercise. For continuous data types, challenges include measurement variance, extreme  
37 observations, and underlying variation structures like blocks. For categorical data, challenges largely center around the  
38 balance or lack thereof between categories. Challenges in the evaluation approach are driven by decision-making about  
39 which data are used for model derivation and which are used for evaluation. We will review these challenges in this  
40 study.

41 **1.3 Model Evaluation**

42 Model evaluation in the context of predictive analytics seeks to explore how well a model can generalize to new  
43 prediction contexts not seen during model training. Although commonly referred to as "model validation" in the  
44 literature, this term implies a false degree of confidence given that the word "validation" means to prove something  
45 true. There is no single test, or recognized suite of tests, to prove a model valid. Instead, the term "evaluation," which  
46 involves assessing the value, nature, character, or quality of something, is more fitting. It is essential to evaluate model  
47 performance on unseen data to ensure the approach is applicable to new experiments. To this end, cross-validation (CV)  
48 is widely recognized as a standard method for model evaluation.

49 The most common CV method is K-fold CV, which partitions the dataset into K equally sized folds. In each iteration,  
 50 one fold is reserved as the test set (i.e., new data, noted as  $\mathcal{D}_{\text{test}}$ ), while the remaining folds are used as the training set  
 51 (noted as  $\mathcal{D}_{\text{train}}$ ) to construct the model. Once the model is trained, it is evaluated on the  $\mathcal{D}_{\text{test}}$  to obtain an estimate of  
 52 the model performance  $\hat{g}$ . The process will iterate K times until each fold has been used as the  $\mathcal{D}_{\text{test}}$  once. The average  
 53 performance over all K folds is deemed as the expected generalization performance of the model  $\mathbb{E}[\hat{g}]$  on new data.

54 However, there is always an evaluation bias between the estimated performance  $\mathbb{E}[\hat{g}]$  and the true generalization  
 55 performance  $G$ , which can only be approximated by evaluating the same model on an infinite number of unseen data.  
 56 Depending on the performance metric used in evaluation, a positive evaluation bias ( $\mathbb{E}[\hat{g}] - G$ ) typically suggests that the  
 57 model evaluation procedure concludes a pessimistic estimation of the model performance, since the true performance  
 58 is expected to be lower than the estimated performance. Another aspect of model evaluation error is the variance of  
 59 each estimated performance  $\hat{g}$  across the K folds. For example, there are five estimates in a 5-fold cross-validation.  
 60 The variance among these five estimates is defined as the evaluation variance. A high evaluation variance suggests that  
 61 the performance is sensitive to the choice of data folds, and a small size or an over-complex model can lead to a high  
 62 evaluation variance.

63 There is a trade-off relationship between the evaluation bias and variance from a squared evaluation bias, the derivation  
 64 of the relationship is shown in the Eq. 23 in the Appendix. When performing K-fold CV with a fixed sample size  
 65 and model complexity, the choice of K is the pivotal element shaping the model evaluation. When the K is set to a  
 66 larger value; each training set  $\mathcal{D}_{\text{train}}$  is larger in size, resulting in a model trained on a more representative subset of the  
 67 population of interest, leading to lower bias. However, a large K comes with a trade-off: the corresponding test subset  
 68  $\mathcal{D}_{\text{test}}$  is compressed in size, making the tested model more sensitive to the specific data points, and thus inflating the  
 69 validation variance. Conversely, a smaller K, along with a minor training set  $\mathcal{D}_{\text{train}}$ , reduces their representativeness and  
 70 increases bias. Nevertheless, a larger size of the test set  $\mathcal{D}_{\text{test}}$  leads to more consistent estimations across the folds and,  
 71 consequently, reduces the validation variance.

72 Leave-one-out cross-validation (LOOCV) is a variant of K-fold CV where K equals the sample size of the complete  
 73 dataset  $\mathcal{D}$ . It provides an unbiased estimation of model performance because the training set  $\mathcal{D}_{\text{train}}$  closely resembles the  
 74 unseen population of interest, given its size of  $N - 1$ , where  $N$  is the sample size. However, as the trade-off discussion  
 75 suggested, this method can lead to high validation variance due to the model being evaluated on one sample at a time.  
 76 The true unbiased nature of LOOCV is fully realized only when all K folds are utilized. Performing an incomplete  
 77 LOOCV can introduce significant bias because of the inherent high validation variance, which often occurs when  
 78 training each model iteration is prohibitively time-consuming or computationally demanding. In specific contexts, such  
 79 as genomic prediction, strategies like the one described by Cheng et al. leverage the matrix inverse lemma, which  
 80 allows for computational savings by avoiding the inversion of large matrices in each fold. This technique significantly  
 81 reduces the dependency of computational resources on the sample size [1]. Van Dixhoorn et al. exemplify the use of  
 82 LOOCV with a small dataset, aiming to predict cow resilience with limited data resources [2]. Nevertheless, for large

83 datasets, LOOCV is generally not recommended due to computational inefficiency. Further details of bias-variance  
84 trade-off have been extensively explored in the statistical literature [3, 4].

85 **1.4 Model Selection**

86 Model selection becomes necessary when models are not entirely determined by the data alone. For example, in a  
87 regularized linear regression model such as a ridge regression [5] or the least absolute shrinkage and selection operator  
88 (LASSO) [6], it is essential to define a regularization parameter,  $\lambda$ , before fitting the model to the data. A larger  $\lambda$  value  
89 yields a more regularized model, which tends to reduce smaller coefficients to negligible values or zero. This approach  
90 helps in preventing overfitting noise in the training data. The definition of loss functions for the regularized models  
91 were described in 25 and 26 of the Appendix.

92 These pre-defined parameters, like  $\lambda$ , influence model fitting and remain constant during the training process. Such  
93 parameters are referred to as hyperparameters. Beyond regularized models, hyperparameters are crucial in other  
94 predictive models, enhancing flexibility and robustness. For example, in the Support Vector Regression (SVR) [7],  
95 the regressors  $X$  are projected onto a linear subspace to approximate the target variable  $Y$ . By choosing a suitable  
96 kernel function, which transforms the regressors into a non-linear space, as a hyperparameter, SVR can more effectively  
97 capture non-linear relationships, thus significantly improving model performance. Another hyperparameter example is  
98 the number of latent variables in the Partial Least Square (PLS) Regression [8], which condenses the original regressors  
99 into a more manageable set of latent variables, reducing multicollinearity issues. Fewer latent variables might lose  
100 significant information from the original regressors, while too many can lead to overfitting. Similarly, in Random Forest  
101 [9], hyperparameters such as tree depth and the number of trees dictate model complexity. The same applies to the  
102 number of hidden layers and the size of filters in convolutional neural networks [10]. All these examples highlight  
103 the fact that selecting the most suitable hyperparameters, which is known as hyperparameter tuning, is crucial for  
104 optimizing model performance. Feature selection is another crucial aspect of model selection. This process involves  
105 fitting the model to a selected subset of the original features, particularly essential in high-dimensional data scenarios  
106 where the number of features exceeds the number of observations, leading to poor model generalization. For instance,  
107 Ghaffari et al. sought to predict health traits in 38 multiparous Holstein cows using a metabolite profiling strategy. Out  
108 of 170 metabolites, only 12 were identified as effective discriminators between healthy and over-conditioned cows  
109 and were thus selected for the predictive model [11]. Therefore, optimizing feature subsets is a vital model selection  
110 strategy that significantly affects model performance. Including the model selection process within the cross-validation  
111 is essential to avoid common pitfalls. The risk of inflated model performance arises when model selection is guided  
112 by results on the test dataset. Even if the chosen model is subjected to k-fold cross-validation afterward, its selection  
113 bias toward the test set can lead to overestimating its efficacy. This issue has been highlighted in statistical literature  
114 [3]. A practical solution is to divide the dataset into training, validation, and test sets. The validation set is then used  
115 for model selection, ensuring the test set remains completely unused during the training phase, thereby providing a  
116 more accurate measure of model performance. For instance, the study by Rovere et al. exemplifies best practices in

117 hyperparameter tuning and feature selection by employing an independent cross-validation step prior to assessing model  
118 performance. This approach enabled the precise selection of relevant spectral bands from the mid-infrared spectrum  
119 and the optimal number of latent dimensions in PLS with Bayesian regression for predicting the fatty acid profile in  
120 milk [12]. Similarly, Becker et al. demonstrated a robust evaluation by using nested cross-validation loops; the inner  
121 loop conducted a grid search for the best hyperparameters in logistic regression, while the outer loop was designed to  
122 evaluate the performance of the resulting optimized model [13]. Both examples underscore the importance of separating  
123 model selection from performance evaluation to ensure the validity and reliability of the results.

124 **1.5 Cross Validation Design with Block Effects**

125 Blocking is an essential approach in experimental design to control for variations that can confound the variable of  
126 interest. For instance, Lahart et al. investigated the dry matter intake of grazing cows using mid-infrared (MIR)  
127 spectroscopy technology across multiple herds under varying experimental conditions [14]. Given the significant  
128 variation between herds, which may contribute to individual differences in both dry matter intake (i.e., response variable)  
129 and MIR spectra (i.e., independent variables), it is crucial to consider the herd as a blocking factor before evaluating the  
130 predictability of dry matter intake using MIR spectra. This consideration should also extend to model evaluation. In the  
131 cited study, variations in dry matter intake, the primary focus of the prediction model, were observed to exceed one  
132 standard deviation among some herds. In cross-validation, if samples from the same herd are assigned to different folds,  
133 with one fold used as the test set, the model is likely to achieve high accuracy. This accuracy may largely result from  
134 explaining the inter-herd variation rather than individual variations in dry matter intake, leading to an overestimation of  
135 model performance. To avoid this pitfall, block cross-validation, where each block (i.e., herd in this example) is used as  
136 a fold, is recommended for unbiased model evaluation. Literature reviews have indicated that block cross-validation  
137 effectively evaluates model performance on external or unseen datasets [15]. In the same study by Lahart et al., three  
138 cross-validation strategies were compared: random cross-validation (Random CV), which randomly assigns samples  
139 to folds; within-herd validation, training and testing the model within each herd; and across-herd validation (Block  
140 CV), where each herd is used as a fold and tested in turn. The results showed that performance estimates in block CV  
141 were noticeably lower than the other two strategies, supporting the hypothesis that ignoring block effects inflates model  
142 performance. Other studies considering block effects, including diet [16], herd [12], and farm location [17, 18], have  
143 shown similar results in cross-validation, demonstrating block CV's effectiveness in evaluating model performance on  
144 external datasets.

145 **1.6 Model Performance Metrics**

146 Model performance metrics serve as quantitative indicators for evaluating model performance. They are critical for  
147 benchmarking various modeling approaches and for evaluating hypotheses underpinning these different approaches.  
148 Choosing appropriate metrics to support hypothesis testing is crucial, as in-ideal selection may lead to overly optimistic  
149 conclusions. Due to the different goals of regression and classification tasks, it is critical to ensure that these different

150 model types are evaluated using different metrics. As such, metrics for regression and classification are discussed  
 151 individually.

152 **1.6.1 Metrics in Regression Tasks**

Table 1: Summary of model performance metrics for regression tasks.

| Metric  | Type            | Scale-invariant | Range          |
|---|-----------------|-----------------|----------------|
| Root mean square error (RMSE)                   | Error-Based     | No              | $[0, \infty]$  |
| Mean absolute error (MAE)                       | Error-Based     | No              | $[0, \infty]$  |
| Root mean squared percentage error (RMSPE)      | Error-Based     | Yes             | $[0, \infty]$  |
| Root mean standard deviation ratio (RSR)        | Error-Based     | Yes             | $[0, \infty]$  |
| Pearson's correlation coefficient ( $r$ )       | Linearity-Based | Yes             | $[-1, 1]$      |
| Coefficient of determination ( $R^2$ )          | Linearity-Based | Yes             | $[-\infty, 1]$ |
| Lin's concordance correlation coefficient (CCC) | Linearity-Based | Yes             | $[-1, 1]$      |

153 Regression models aim to predict continuous variables and are commonly employed in diverse applications, such as  
 154 estimating body condition scores [19, 20], body weight [21, 22], milk composition [12, 18, 23, 24], efficiency of feed  
 155 resource usage [16, 25, 26], and early-lactation behavior [2]. The metrics in regression tasks evaluate the agreement  
 156 between the predicted value  $\hat{y}$  and the true values  $y$ . The agreement can be generally quantified in two ways: error-based  
 157 metrics and linearity-based metrics. The metrics are summarized in Table 1.

158 Error-based metrics focus on the deviation of each pair of predicted and true values, while linearity-based metrics  
 159 consider overall linear relationships between the predictions and the truths. The root mean square error (RMSE) and the  
 160 mean absolute error (MAE) are two common error-based metrics:

$$\text{RMSE} = \sqrt{\frac{1}{n} \sum_{i=1}^n (y_i - \hat{y}_i)^2} \quad (1)$$

$$\text{MAE} = \frac{1}{n} \sum_{i=1}^n |y_i - \hat{y}_i| \quad (2)$$

161 where  $y_i$  and  $\hat{y}_i$  are the true and predicted values, respectively, and  $n$  is the sample size. Both metrics preserve the scale  
 162 of the original data, making them easy to interpret in real-world units. Additionally, compared to MAE, RMSE penalizes  
 163 large errors more due to the squared term, making it more sensitive to outliers. In the cow production, monitoring  
 164 animal body weight is a common practice to aid in the management of dairy cows. Studies by Song et al. and Xavier et  
 165 al. have utilized RMSE to assess the effectiveness of three-dimensional cameras in estimating dairy cow body weight,  
 166 yielding RMSE values of 41.2 kg and 12.1 kg, respectively [21, 22]. These figures provide a straightforward value for  
 167 farmers to gauge whether the prediction error is tolerable, considering their specific operational costs and management  
 168 thresholds. In essence, RMSE translates complex model accuracy into practical insights for productive agricultural  
 169 units. When evaluating the same model across different traits, which may have different scales, a common practice is to  
 170 express error metrics in a scale-free manner. This can be achieved by expressing RMSE as a percent of the deviation

171 from the observed value, such as root mean squared percentage error (RMSPE), or as a Root Mean Standard Deviation  
 172 Ratio (RSR) that normalizes the RMSE by the standard deviation of the observed values:

$$\text{RMSPE} = \sqrt{\frac{1}{n} \sum_{i=1}^n \left( \frac{y_i - \hat{y}_i}{y_i} \right)^2} \quad (3)$$

$$\text{RSR} = \frac{\text{RMSE}}{\sigma_y} \quad (4)$$

173 where  $\sigma_y$  is the standard deviation of the observed values. When expressed as a percent, RMSPE typically ranges from  
 174 0 and above, with values closer to 0 indicating perfect prediction. Much like expressing RMSE as a percent, RSR is  
 175 valuable to interpret RMSE in terms of the context of the variance in the observations. Values below 1 suggest that the  
 176 model yields predictions less variable than the standard deviation, while values above 1 suggest that the prediction is  
 177 imprecise.

178 On the other hand, Pearson's correlation coefficients ( $r$ ) and the coefficient of determination ( $R^2$ ) are two common  
 179 linearity-based metrics:

$$\begin{aligned} r &= \frac{\text{cov}(y, \hat{y})}{\sigma_y \sigma_{\hat{y}}} \\ &= \frac{\sum_{i=1}^n (y_i - \bar{y})(\hat{y}_i - \bar{\hat{y}})}{\sqrt{\sum_{i=1}^n (y_i - \bar{y})^2 \sum_{i=1}^n (\hat{y}_i - \bar{\hat{y}})^2}} \end{aligned} \quad (5)$$

$$\begin{aligned} R^2 &= 1 - \frac{SS_{\text{residual}}}{SS_{\text{total}}} \\ &= 1 - \frac{\sum_{i=1}^n (y_i - \hat{y}_i)^2}{\sum_{i=1}^n (y_i - \bar{y})^2} \end{aligned} \quad (6)$$

180 where  $SS_{\text{residual}}$  is the residual sum of squares and  $SS_{\text{total}}$  is the total sum of squares. Each  $y_i$  and  $\hat{y}_i$  are the  $i$ th elements  
 181 of the actual response vector  $y$  and the predicted response vector  $\hat{y}$ , respectively.  $\bar{y}$  and  $\bar{\hat{y}}$  are their respective means.  
 182 Both  $r^2$  and  $R^2$  are scale invariant, meaning their values are unaffected by the scale of the observed data because they  
 183 are normalized by the variation in the denominator.

184 The correlation coefficient  $r$  measures the strength of the linear relationship between two continuous variables,  $y$  and  $\hat{y}$ ,  
 185 and ranges from -1 to 1. A value of 0 indicates no prediction accuracy in the evaluated model. One special characteristic  
 186 of correlation  $r$  is that it is unaffected by the scale of the predictions or biases; it focuses on the relative changes  
 187 in the predicted values compared to the true values. Thus, even if the prediction biases are scaled up or down, the  
 188 correlation  $r$  between  $\hat{y}$  and  $y$  remains the same. This property is particularly useful when the focus is more on ranking  
 189 predictions rather than their absolute values. For example, this metric has been used to evaluate models that identify  
 190 high-performing production individuals, demonstrating the ability to predict nutrient digestibility in dairy cows [26] and  
 191 to select models based on their ability to rank traits such as feed intake and milk composition in dairy cows [27, 12].

192 The coefficient of determination  $R^2$  quantifies model performance from the proportion of variance in the dependent  
 193 variable that is predictable from the independent variables. It ranges from negative infinity to 1, where 1 indicates  
 194 that the model explains all the variance in the dependent variable, and 0 indicates that the model performs no better  
 195 than predicting all samples as the mean of the observed values.  $R^2$  is useful in comparing multiple regression models,  
 196 as demonstrated in studies that regress body weight of dairy cows on a set of morphological traits [22], examine  
 197 the relationship between milk spectral profiles and nitrogen utilization efficiency [16], and evaluate the predictive  
 198 performance of milk fatty acid composition [23].

199 It worth noting that many literatures have misinterpreted the relationship between  $r$  and  $R^2$ . The coefficient of  
 200 determination  $R^2$  is not always equivalent to the square of the correlation coefficient  $r^2$ . The equivalence only holds  
 201 when the same dataset is used for both model fitting and evaluation in a least squares regression model. The model  
 202 assumes a zero covariance between the fitted residual and the predicted values  $\hat{y}$ , and it also assumes that the residuals  
 203 (i.e., prediction biases) are centered on zero. In practice when predictions are made on new data, those assumptions  
 204 are often violated, leading to discrepancies between  $r^2$  and  $R^2$ . A details derivation of the equivalence is provided in  
 205 Equation 27 28 in the Appendix.

206 In addition to  $r^2$  and  $R^2$ , another linearity-based metric is Lin's concordance correlation coefficient (CCC) [28]:

$$\begin{aligned} \text{CCC} &= \frac{2r\sigma_y\sigma_{\hat{y}}}{\sigma_y^2 + \sigma_{\hat{y}}^2 + (\bar{y} - \hat{\bar{y}})^2} \\ &= \frac{2\text{cov}(y, \hat{y})}{\sigma_y^2 + \sigma_{\hat{y}}^2 + (\bar{y} - \hat{\bar{y}})^2} \end{aligned} \quad (7)$$

207 where  $r$  is the Pearson correlation coefficient. The CCC is a comprehensive metric because it considers both the  
 208 correlation and the scale bias between the predicted and true values. It fills the gap left by  $r^2$  where the scale bias is  
 209 ignored. Geometrically, CCC measures how well the predicted values  $\hat{y}$  fall on the 45-degree line in a scatter plot of  
 210 the predicted (x-axis) and true values (y-axis). It is advantageous over  $R^2$  because it consistently ranges from -1 to 1,  
 211 making it easier to interpret and compare across different studies. The CCC is crucial when precise predictions are  
 212 required for both the scale and the rank of the trait of interest, such as in studies predicting cotton crop yields based on  
 213 soil and terrain profiles [29].

### 214 1.6.2 Metrics in Classification Tasks

215 Classification models aim to predict categorical outcomes such as 'healthy' or 'sick,' 'susceptible' or 'resistant,' and  
 216 'high yield' or 'low yield.' To evaluate classification performance, one must first establish a confidence threshold to  
 217 dichotomize the prediction probabilities. For instance, if a prediction probability exceeds the threshold, the sample is  
 218 predicted as a positive sample. It is worth mentioning that this threshold is adjustable to fine-tune model performance  
 219 for particular uses. The discussed metrics in classification tasks are summarized in Table 2.

Table 2: Summary of model performance metrics for classification tasks.

| Metric   | Label-invariant | Threshold-independent |
|--|-----------------|-----------------------|
| Accuracy   | No              | No                    |
| Precision  | No              | No                    |
| Recall   | No              | No                    |
| F1 score   | No              | No                    |
| Matthews correlation coefficient (MCC)                           | Yes             | No                    |
| Area under the precision-recall curve (AUC-PR)                   | No              | Yes                   |
| Area under the receiver operating characteristic curve (AUC-ROC) | Yes             | Yes                   |
| Area under the MCC curve (AUC-MCC)                               | Yes             | Yes                   |

220 Accuracy is the most straightforward metric for evaluating classification models:

$$\text{Accuracy} = \frac{\text{Total Correct Predictions}}{\text{Total Predictions}} = \frac{\text{TP} + \text{TN}}{\text{TP} + \text{TN} + \text{FP} + \text{FN}} \quad (8)$$

221 where TP, TN, FP, and FN represent the number of true positives, true negatives, false positives, and false negatives,  
 222 respectively. It summarizes an overall model performance by calculating the proportion of correctly classified samples  
 223 among all samples. Nonetheless, accuracy can be misleading when the classes are imbalanced. For example, if a study  
 224 predicting the presence of a specific event, of which the prevalence was only 10%. In this case, a model that predicts all  
 225 samples as negative would achieve an accuracy of 90%, which is misleadingly high. To address this issue, precision and  
 226 recall are introduced:

$$\text{Precision} = \frac{\text{TP}}{\text{Total Predicted Positives}} = \frac{\text{TP}}{\text{TP} + \text{FP}} \quad (9)$$

$$\text{Recall} = \frac{\text{TP}}{\text{Total Actual Positives}} = \frac{\text{TP}}{\text{TP} + \text{FN}} \quad (10)$$

$$\text{F1} = 2 \times \frac{\text{Precision} \times \text{Recall}}{\text{Precision} + \text{Recall}} \quad (11)$$

227 Precision and recall refine the assessment of a classification model by offering insights that accuracy alone may  
 228 overlook. Precision calculates the fraction of true positives among all positive predictions, essentially measuring  
 229 the trustworthiness of positive predictions made by the model (Eq. 9). High precision is crucial in scenarios where  
 230 false positives incur significant costs, and false negatives are more tolerable. For instance, in contexts where clinical

treatments and culling are expensive, such as detecting bovine tuberculosis [30] or mastitis [31] using non-invasive methods, a high-precision model is crucial to minimize unnecessary costs and interventions from false positives. On the other hand, recall, also known as sensitivity, quantifies the ratio of true positives to all actual positives, assessing the model's ability to identify positive cases (Eq. 10). High recall is essential where missing a positive case has serious consequences, or where false positives are easily rectifiable. For instance, detecting lameness or abnormal gait is crucial, as these can indicate underlying pathologies [32] and impact welfare-related transport decisions [33]. An automated detection system [32, 34, 35] with high recall can mitigate economic losses by flagging at-risk cows. The benefit here lies in the feasibility of re-examining false positives, thus preventing more severe outcomes from undetected cases. Lastly, the F1 score, which is the harmonic mean of precision and recall, provides a balanced measure of model performance (Eq. 11). It is usually used as an overall performance metric when precision and recall are equally important.

However, it is worth emphasizing that precision and recall focus predominantly on positive samples. Inappropriately assigning a predominant background event as the positive class can lead to skewed interpretations. Hence, the Receiver Operating Characteristic (ROC) curve provides an another crucial tool for assessing a model's performance in a label-agnostic manner, meaning it is not biased by the class distribution as precision and recall are. An ROC curve plots one minus specificity against sensitivity. The equations for specificity and sensitivity are as follows:

$$\begin{aligned} \text{Specificity} &= \frac{\text{TN}}{\text{Total Actual Negatives}} \\ &= \frac{\text{TN}}{\text{FP} + \text{TN}} \end{aligned} \tag{12}$$

$$\begin{aligned} \text{Sensitivity} &= \text{Recall} \\ &= \frac{\text{TP}}{\text{Total Actual Positives}} \\ &= \frac{\text{TP}}{\text{TP} + \text{FN}} \end{aligned} \tag{13}$$

A model's effectiveness, as depicted on the ROC curve, is gauged by how closely a point on the curve approaches the top-left corner. A steep ascent from the left side of the curve signifies the model's ability to correctly identify most true positives while incurring a low rate of false positives. A random guess, with a 50% chance of correct prediction, corresponds to a diagonal line on the ROC curve. In dairy science, the ROC curve has been extensively utilized, for example, in predicting mastitis from milk composition [36] and diagnosing pregnancy using spectroscopy technology [37]. In this hypothetical example, the ROC curve also demonstrates robustness and label-invariance with a consistent AUC of 0.875, regardless of whether the original or inverted labels are used.

254 In addition to the metrics, the Matthews Correlation Coefficient (MCC) provides a symmetrical measure of the quality  
 255 of binary classifications. The MCC considers both positive and negative samples in the dataset, providing a balanced  
 256 measure of a model's performance [38]. It is defined as:

$$\text{MCC} = \frac{\text{TP} \times \text{TN} - \text{FP} \times \text{FN}}{\sqrt{(\text{TP} + \text{FP})(\text{TP} + \text{FN})(\text{TN} + \text{FP})(\text{TN} + \text{FN})}} \quad (14)$$

257 The equation 14 symmetrically incorporates all four components of TP, TN, FP, and FN). This symmetry makes MCC  
 258 invariant to class distribution changes. The coefficient ranges from -1 to 1, where 1 indicates perfect classification,  
 259 0 indicates no better performance than random guessing, and -1 signifies total disagreement between prediction and  
 260 observation. In a case study that used feeding and daily activity behaviors to diagnose Bovine Respiratory Disease  
 261 in dairy calves, MCC proved particularly insightful [39]. The models in this study exhibited strong performance on  
 262 negative samples (i.e., healthy calves), which were more prevalent, resulting in high specificity. However, sensitivity  
 263 was relatively low at 0.54. In this context, MCC, with a value of 0.36, provided a more nuanced and representative  
 264 measure of model performance, especially given the skew towards negative samples.

## 265 1.7 Study Objectives

266 This simulation study aims to highlight how biased or over-optimistic estimations of model performance usually come  
 267 from inappropriately conducting CV, a technique crucial for characterizing expected model performance on “new”  
 268 data. We demonstrate how common pitfalls, including using the exact data for both training and model assessment,  
 269 excluding the model selection process from CV, and neglecting experimental block effects, contribute to challenges  
 270 in model evaluation. Further, we scrutinize common metrics used in evaluating prediction models, including those  
 271 used for regression and classification tasks. Because no single metric provides a comprehensive perspective of model  
 272 performance, we seek, through this work, to highlight the importance of understanding the underlying theory of each  
 273 metric to avoid misleading conclusions.

274 There are five simulation studies being conducted to address these challenges. The first simulation study will focus  
 275 on the bias-variance trade-off in CV, demonstrating how the choice of K in K-fold CV affects the evaluation bias and  
 276 variance. The second simulation study will investigate the impact of mistakenly using the same data for model selection  
 277 and evaluation, highlighting the inflated model performance. The third simulation study will explore the effect of  
 278 excluding block effects in CV, demonstrating how ignoring block effects can lead to over-optimistic model performance.  
 279 The fourth simulation study will present four hypothetical predictions made in the same regression tasks, leading to  
 280 different interpretations with different metrics. The fifth simulation study will demonstrate the impact of imbalanced  
 281 data on classification model evaluation, showing how the choice of metrics can lead to misleading conclusions. Overall,  
 282 this series of simulation studies aims to guide researchers in accurately and consistently reporting model performance,  
 283 thereby supporting integrity and scientific rigor in prediction modeling research.

<sup>284</sup> **2 Materials and Methods**

<sup>285</sup> **2.1 Study 1: Evaluation bias and variance of cross-validation**

<sup>286</sup> This study investigated the interplay between sample size and various performance estimators and their collective  
<sup>287</sup> impact on bias and variance during model evaluation. It is hypothesized that increasing the sample size will reduce  
<sup>288</sup> both bias and variance. Additionally, it is expected that the validation variance will increase with the number of folds  
<sup>289</sup> in the CV, while simultaneously reducing bias. Since K-fold CV employs a fraction (i.e.,  $K - 1$  folds) of the data  
<sup>290</sup> for training, it may provide a pessimistic estimate of model performance. Hence, this study designed to assess the  
<sup>291</sup> underestimation from each performance estimators, including K-fold CV with K set to 2, 5, and 10, as well as LOOCV  
<sup>292</sup> where K equals the sample size N, and the "In-Sample" evaluation, which assesses model performance on the same  
<sup>293</sup> dataset used for training, potentially leading to an overly optimistic bias. To gauge model performance, three metrics  
<sup>294</sup> are employed: RMSE (Eq. 1), r (Eq. 5), and  $R^2$  (Eq. 6). The validation model is a multivariate linear regression with  
<sup>295</sup> ten input features and one output target, all drawn from a standard normal distribution  $\mathcal{N}(0, 1)$ , implying no expected  
<sup>296</sup> linear relationship between inputs and the target, with an expected correlation r of zero. The sample sizes N are varied  
<sup>297</sup> among 50, 100, and 500 to explore the dynamics between sample size and performance estimators. Each configuration  
<sup>298</sup> is repeated across 1000 iterations to assess the distribution of bias and variance.

<sup>299</sup> For each iteration, the dataset  $\mathcal{D} = (X, Y)$  was sampled as per the simulation's premise. In the case of K-fold CV, the  
<sup>300</sup> dataset  $\mathcal{D}$  was partitioned into K folds in which each fold is  $\mathcal{D}_k = (X_k, Y_k)$ . For the "In-Sample" approach, partitioning  
<sup>301</sup> does not occur. The linear model f is trained on the training set  $\mathcal{D}_{-k}$  (denoted as  $f_{\mathcal{D}_{-k}}$ ) to estimate regression coefficients  
<sup>302</sup>  $\beta$ , which then predicts the target variable  $\hat{Y}_k$  from the test set  $\mathcal{D}_k$ . The procedure of K-fold CV can be expressed as:

$$\begin{aligned} \text{Training: } & Y_k = f_{\mathcal{D}_{-k}}(X_k) + \epsilon \\ & = X_k\beta + \epsilon \\ \text{Testing: } & \hat{Y}_k = f_{\mathcal{D}_{-k}}(X_k) \\ & = X_k\beta \quad k = 1, 2, \dots, K \end{aligned} \tag{15}$$

<sup>303</sup> For the "In-Sample" performance estimator, predictions were made without splitting, as:

$$\begin{aligned} \text{Training: } & Y = f_{\mathcal{D}}(X) \\ & = X\beta + \epsilon \\ \text{Testing: } & \hat{Y} = f_{\mathcal{D}}(X) \\ & = X\beta \end{aligned} \tag{16}$$

304 Where:

- 305 •  $X$  denotes the input regressors sampled from a standard normal distribution  $\mathcal{N}(0, 1)$  with dimensions  $N \times 10$ .
- 306 •  $Y$  denotes the target variable sampled from a standard normal distribution  $\mathcal{N}(0, 1)$  with dimensions  $N \times 1$ .
- 307 •  $X_{-k}$  and  $Y_{-k}$  are the input regressors and target variable in the training set  $\mathcal{D}_{-k}$ .
- 308 •  $X_k$  denotes the input regressors in the test set  $\mathcal{D}_k$ .
- 309 •  $\hat{Y}_k$  denotes the predicted target variable in the test set  $\mathcal{D}_k$ .
- 310 •  $\beta$  denotes the estimated regression coefficient with dimensions  $10 \times 1$ .
- 311 •  $\epsilon$  denotes the error term assumed to be normally distributed.

312 Estimated performance  $\mathbb{E}[\hat{g}(f_{\mathcal{D}})]$  was derived by averaging the performance metrics across all K folds as per Eq. 20.  
 313 The bias and variance of the evaluation were calculated using Eqs. 21 and 22, respectively. To approximate true  
 314 model performance  $G(f_{\mathcal{D}})$ , a hundred unseen datasets  $\mathcal{D}^*$  were generated identically to  $\mathcal{D}$ , and the performance  $G(f_{\mathcal{D}})$   
 315 was estimated by averaging the performance metrics across all  $\mathcal{D}^*$ . The detailed steps to compute evaluation bias and  
 316 variance are provided in the supplementary materials.

## 317 2.2 Study 2: Model Selection in Cross-Validation

318 The objective of this simulation study is to examine the effect of improper model selection implementation on validation  
 319 bias. The focus will be on the model selection procedures of feature selection and hyperparameter tuning. The study  
 320 hypothesizes that utilizing the test set inappropriately during any model selection stage will lead to a significant  
 321 overestimation of model performance. This study simulated a regression task using an SVR model, which utilized  
 322 various kernel functions to project a subset of features, X, to predict a target variable, Y. Both X and Y are drawn from  
 323 a normal distribution  $\mathcal{N}(0, 1)$  to establish a baseline null correlation (performance r=0) for assessing validation bias.  
 324 This study set the sample size and number of features at 100 and 1000, respectively. Feature selection is executed by  
 325 choosing the top 50 features that correlate most strongly with Y. For hyperparameter tuning, four kernel functions were  
 326 evaluated: linear, polynomial, radial basis function, and sigmoid.

327 This study introduces notations FS for feature selection and HT for hyperparameter tuning, assigning a binary indicator  
 328 (0 or 1) to denote incorrect (0) or correct (1) implementation of model selection. This yields four possible combinations  
 329 of model selection strategies: “FS=0; HT=0”, “FS=0; HT=1”, “FS=1; HT=0”, “FS=1; HT=1” (Figure 1). When  
 330 FS=0, feature selection precedes cross-validation splitting. If FS=1, feature selection occurs within each fold of the  
 331 training set during cross-validation. With hyperparameter tuning, a correct implementation (HT=1) involves splitting  
 332 the dataset into training (64%), validation (16%), and test (20%) sets. The model is trained and tuned using the training  
 333 and validation sets, respectively, while the test set is reserved for a single evaluation of model performance. Conversely,  
 334 with HT=0, only training (80%) and test (20%) sets are used, risking validation bias as the test set informs both  
 335 training and performance reporting. A 5-fold cross-validation approach was deployed for all strategies. Validation

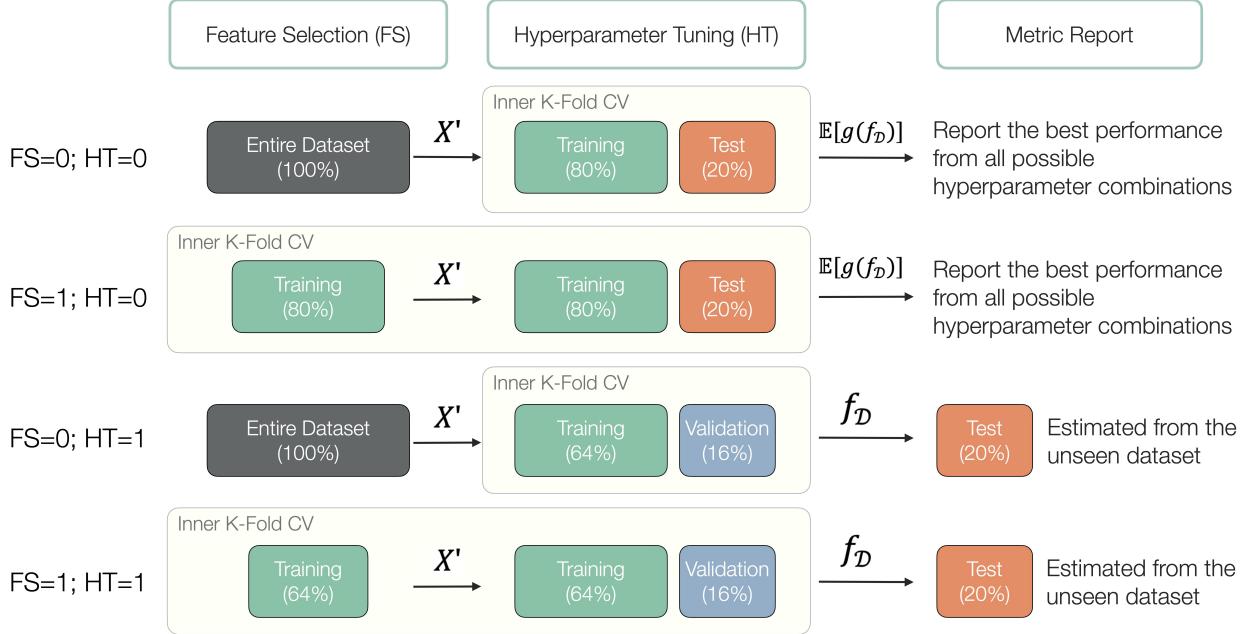


Figure 1: Workflow diagram illustrating four cross-validation strategies of feature selection (FS) and hyperparameter tuning (HT), where 0 denotes incorrect implementation and 1 indicates correct practice.  $X'$  is the selected feature subset,  $\mathbb{E}[\hat{g}(f_D)]$  is the expected generalization performance,  $f_D$  is the model trained on the training set without being revealed to the test set.

336 bias is measured as the discrepancy between the model selection-influenced performance estimate and the expected  
 337 generalization performance ( $r=0$ ), using the Pearson correlation coefficient between predicted and observed values.  
 338 Over 1000 sampling iterations, the study assesses the distribution of validation bias. A t-test will determine whether the  
 339 validation bias significantly deviates from zero.

### 340 2.3 Study 3: Block Effects in Cross-Validation

341 The objective of the study is to demonstrate how a Random CV, which randomly assigns the samples to folds without  
 342 considering the block effects, could overestimate the model performance. This study also conducts a block CV, where  
 343 each block is used as a fold in the cross-validation, as the benchmark. The hypothesis is that the model performance  
 344 estimated by Random CV is significantly higher than the estimation by block CV. This study simulated a regression  
 345 task with 100 instances across ten features, denoted as  $X$ , and one single response variable,  $Y$ . Both  $X$  and  $Y$  are  
 346 derived from a standard normal distribution. To introduce a block factor, the study groups every 20 observations into a  
 347 block, with each block incrementally increasing by  $b$  units from zero, where  $b$  was simulated from 0.5 to 3.0 with an  
 348 increment of 0.5. Within these ten features, one is substituted as the block level, represented by an integer from 0 to 4,  
 349 augmented with random noise drawn from a standard normal distribution. This setup aims to simulate a scenario where  
 350 the predictors primarily capture block variation, given the null expectation in predictability when using ten random  
 351 variables  $X$  to forecast another random variable  $Y$ . The study investigates two model evaluation strategies: Block CV  
 352 and Random CV, both utilizing a 5-fold cross-validation method. In block CV, each block serves as a separate fold,

353 while in Random CV, samples are randomly allocated to each fold (Figure 2). The predictive model is linear regression,  
 354 and the performance is evaluated using Pearson's correlation coefficient. This simulation runs for 1000 iterations, with  
 355 X and Y being resampled in each cycle. A one-tailed t-test assesses if the mean estimated performance significantly  
 356 exceeds zero. Additionally, an Analysis of Variance (ANOVA) table is calculated when b is 0.5 to ascertain if the  
 357 simulated block variation notably exceeds the assumed individual variation, representing the primary interest.

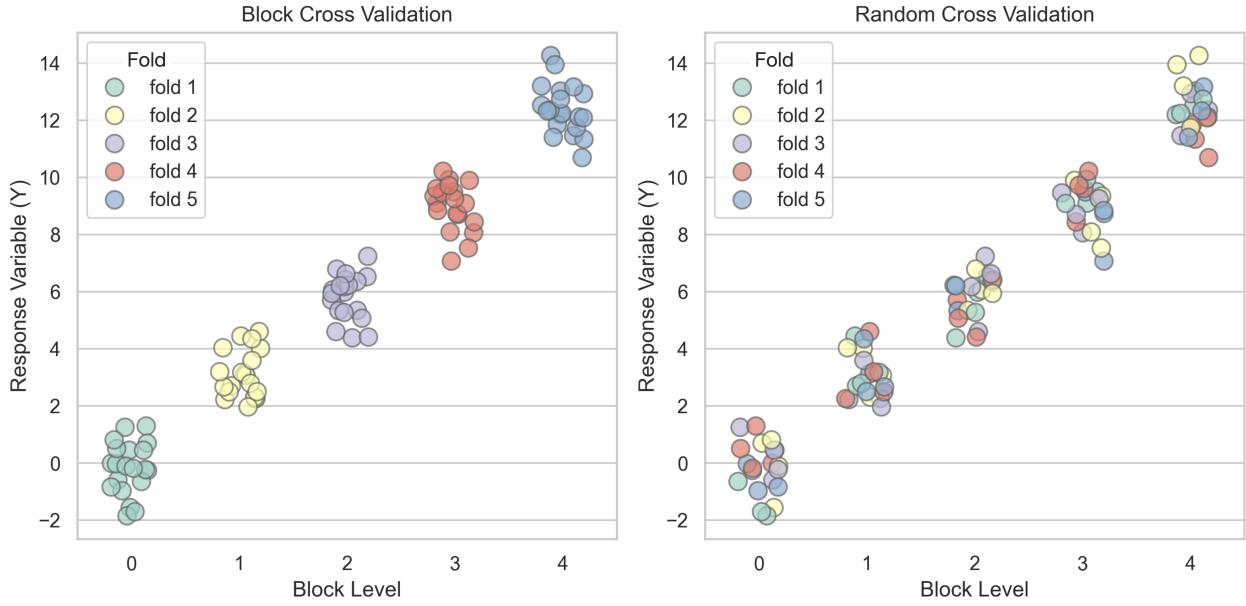


Figure 2: Illustration of fold assignment in block cross validation (left) and random cross validation (right). Folds are color-coded, and the block effect is set to 3 in this example.

#### 358 2.4 Study 4: Performance Metrics in Regression Tasks

359 This study explores two error-based metrics, Root Mean Squared Error (RMSE) and Root Mean Squared Percentage  
 360 Error (RMSPE), and three linearity-based metrics, Pearson Correlation Coefficient ( $r$ ), the Coefficient of Determination  
 361 ( $R^2$ ), and the Concordance Correlation Coefficient ( $CCC$ ), in a variety of commonly-encountered data challenges.  
 362 These data challenges are depicted through 4 scenarios, representing data commonly encountered in predictive  
 363 applications varying in scope (scenarios "Baseline" and "Scaled"), data with outliers disrupting the scale of prediction  
 364 (scenario "Outlier Focused"), and data with an underlying grouping structure (scenario "Clustered"). The statistical  
 365 description of the approach to generating each of these scenarios is included below. Practical examples of real-world  
 366 instances of these types of data challenges are also described.

367 In the hypothetical example depicted in Figure 7, 100 observations were generated from two separate normal  
 368 distributions. The first 50 observations were drawn from a normal distribution with a mean of -3 and a standard  
 369 deviation of 1, denoted as  $\mathcal{N}(-3, 1)$ . The remaining 50 observations were generated from another normal distribution,  
 370  $\mathcal{N}(3, 1)$ . Utilizing two distinct distributions served to simulate experimental block effects, preset at a magnitude of 6

371 units for this experiment. Based on the simulated observations, four scenarios of predictions were derived according to  
372 the setting below:

- 373     • Scenario "Baseline": To establish a correlation relationship, the observations were added another random  
374       variable sampled from  $\mathcal{N}(0, 1)$  to introduce prediction errors. This scenario represents a “best case” for  
375       developing predictive analytics, and could be exemplary of scenarios like predicting a scaled performance  
376       response (i.e., milk yield, average daily gain) from measurable input variables like dry matter intake, sensor  
377       system data, or past performance data.
- 378     • Scenario "Scaled": The prediction outcome from Scenario "Baseline" was multiplied by 5, simulating  
379       predictions with a larger variance while maintaining the same relative order as the original predictions. There  
380       are some responses that have naturally greater proportional variation compared with others. For example,  
381       an animal’s body core temperature is unlikely to vary by more than 5%; however, daily variation around  
382       measurements like feed intake can range upwards of 30 to 40%. Comparison of scenarios "Baseline" and  
383       "Scaled" explore how this natural variation should be included in interpreting predictive analytics.
- 384     • Scenario "Outlier Focused": only the top 10% of predictions that deviate the most from zero in Scenario  
385       "Baseline" were raised to the power of 3. The rest of the predictions were set to zero. This scenario simulates  
386       a prediction that focuses solely on the extreme samples. In disciplines like nutritional exploration, the  
387       emphasis of predictive analytics typically focuses on understanding the mean animal or the mean response  
388       of an individual animal; however, in predictive analytics focused on health or genetic merit, the emphasis of  
389       prediction is often on the extreme observations. Analytics to understand the extreme observations is always  
390       complicated by the question of whether extremes are due to true outliers or some sort of measurement error.  
391       As precision livestock farming advances, the opportunities for measurement error due to erroneous sensor  
392       measurements increases.
- 393     • Scenario "Clustered": Values sampled from two normal distributions,  $\mathcal{N}(-3, 2)$  and  $\mathcal{N}(3, 2)$ , were added  
394       respectively to the predictions made in Scenario "Baseline" of Block A (cross markers in Figure 7) and  
395       Block B (circle markers in Figure 7). In the animal sciences we often rely on blocks as an experimental  
396       tool to support analytics given challenging experimental design or constrained animal units. Many times,  
397       the difference between blocks dwarfs the differences observed within a block, resulting in a masking of true  
398       effects due to the block influence. This scenario amplified the original block effects, simulating a model that  
399       effectively distinguished between different blocks (e.g., herd or breed) but was less capable of predicting  
400       individual variations within each block. An example of this scenario might be simulating milk production  
401       or body weight across species – the magnitude of the difference between sheep and cattle (for example) far  
402       outweighs the magnitude of the difference of sheep or cattle over time.

403 This quartet of predictions serves to simulate potential challenges and complexities encountered in real-world modeling  
404 scenarios, thereby providing a foundation for evaluating different performance metrics used in regression problems.

**405 2.5 Study 5: Performance Metrics in Classification Tasks**

406 This study presents a hypothetical example to highlight how the choice of different performance metrics can lead to  
407 different interpretations of a model's effectiveness. The example focuses on binary classification, where the outcome is  
408 either positive ( $Y=1$ ) or negative ( $Y=0$ ). Suppose a binary classification model always outputs a probability between 0  
409 and 1, indicating the likelihood that a sample belongs to the positive class. This example assumes that the model has  
410 high confidence in correctly predicting 1 out of 4 positive and 5 out of 6 negative samples. This example intends to  
411 illustrate a scenario where the positive outcome is rare, such as predicting the onset of a calving event in dairy cows  
412 [40, 41]. The example data is shown in Figure 8. In addition to the original labels, this example also examines a  
413 scenario with inverted labels (Figure 8. Upper). Since most classification metrics prioritize positive samples, it is  
414 generally advisable to designate the event of interest as the positive class in binary classification problems. Inverting  
415 the labels illustrates the potential overestimation of model performance when the more common, but less significant,  
416 background event is mistakenly marked as the positive class. It is important to note that inverting the labels in this  
417 example only affects the interpretation of model performance, not the model configuration or parameters. To evaluate  
418 classification performance, one must first establish a confidence threshold to dichotomize the prediction probabilities.  
419 For instance, if a prediction probability exceeds the threshold, the sample is labeled positive. By default, the threshold  
420 is set at 0.5 for its simplicity. For example, in the third data row of the example data: With a prediction probability  
421 of 0.38 that falls below the threshold, the sample is deemed negative, resulting in a false negative classification since  
422 the ground truth is positive. It is worth mentioning that this threshold is adjustable to fine-tune model performance for  
423 particular uses. A confusion matrix (Figure 8. Lower), effectively encapsulates prediction outcomes. The rows in this  
424 2x2 matrix correspond to ground truth, while its columns reflect predictions. Correct predictions populate the diagonal  
425 cells, and errors fill the off-diagonal ones. This matrix serves as the foundation for computing various metrics to assess  
426 model performance, which will be explored in the result sections.

427 **3 Results and Discussion**

428 **3.1 Study 1: The Impact of Estimator Choice and Sample Size on Model Evaluation Reliability**

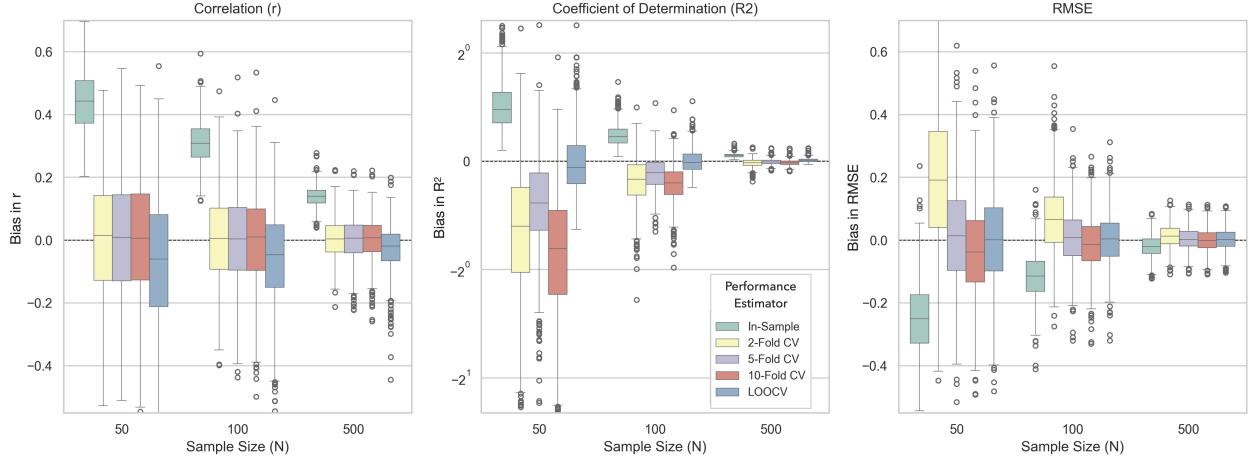


Figure 3: Simulation results of evaluation bias from 1000 sampling iterations. Multiple performance estimators across different sample sizes were color-coded. Three metrics:  $r$ ,  $R^2$ , and RMSE, were displayed in the column facets.

429 The simulation results, depicted in box plots (Figure 3 and 4), explored the evaluation bias and variance distribution.  
 430 Figure 3 examines the bias alterations across various estimators and sample sizes. Independent of the estimator and  
 431 metric, the bias diminishes with increasing sample sizes. The in-sample estimator consistently overestimates across all  
 432 metrics and sample sizes, underscoring the necessity of CV for unbiased performance evaluation. In CV estimators,  
 433 although LOOCV is traditionally viewed as unbiased, it shows underestimation in model performance, especially when  
 434 the metric is correlation coefficient ( $r$ ). Comparatively, 2-, 5-, and 10-fold CV provide a more unbiased estimation  
 435 than LOOCV for all sample sizes. However, for metrics like  $R^2$  or RMSE, LOOCV emerges as the least biased  
 436 estimator. While K-fold CV exhibits higher bias than LOOCV, this difference dwindles when the sample size exceeds  
 437 500. Notably, 10-fold CV, contrary to expectations, demonstrates higher bias than 5-fold CV for small sample sizes (50  
 438 and 100) in the  $R^2$  metric, though this disparity also becomes insignificant at larger sample sizes.  
 439 Considering LOOCV's singular data point testing, its evaluation variance is pertinent only for RMSE, which permits  
 440 single data point evaluations. Figure 4 illustrates the bias and variance in RMSE across different performance estimators  
 441 as a function of sample size  $N$ . Both bias and variance in RMSE decrease as sample size increases, aligning with the  
 442 hypothesis. LOOCV provides the least biased estimation, while 2-fold CV exhibits the highest bias without significant  
 443 reduction at larger sample sizes. However, biases across all estimators converge at a sample size of 500. In terms of  
 444 evaluation variance, LOOCV consistently shows higher values than other estimators for all sample sizes. Additionally,  
 445 a lower number of folds  $K$  correlates with reduced variance, which is also in line with the hypothesized trend.

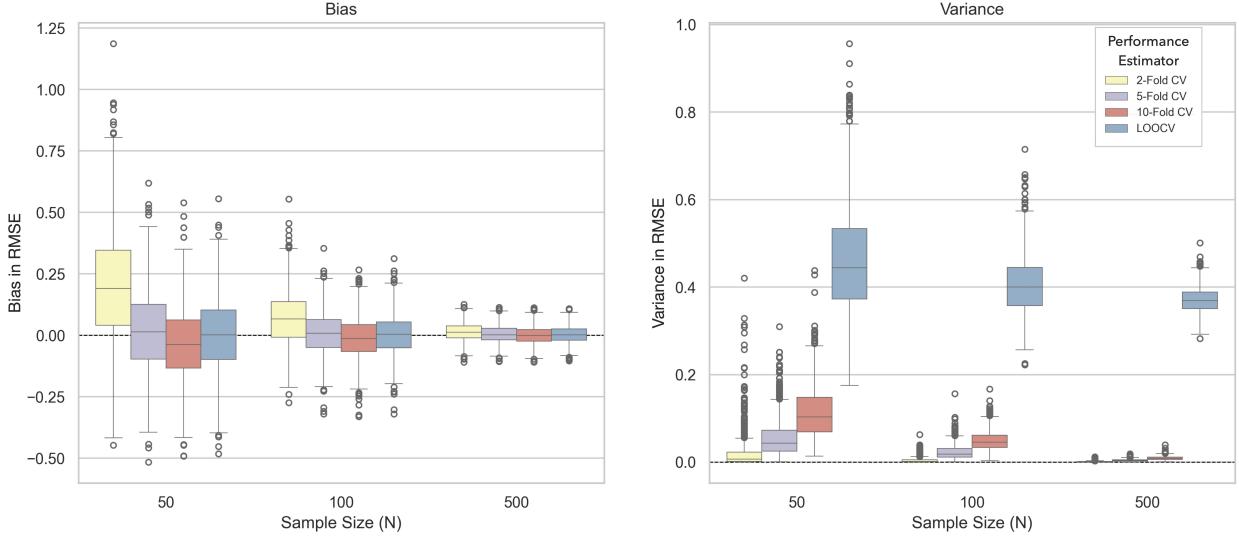


Figure 4: Simulation results of evaluation bias and variance from 1000 sampling iterations. Multiple performance estimators across different sample sizes were color-coded. Only RMSE was displayed. Bias and variance were listed in the left and right facets, respectively.

446 In conclusion, when conducting model evaluation, it is crucial to consider the estimator and sample size, as they  
 447 significantly influence evaluation reliability which can be decomposed into bias and variance. Larger sample sizes  
 448 generally lead to reduced bias and variance, enhancing the reliability of the evaluation process. For unbiased performance  
 449 estimation, CV methods, such as K-fold CV and LOOCV, are preferable to in-sample estimation. LOOCV often  
 450 provides less biased estimations for certain metrics but can exhibit higher variance. It is also noteworthy that the number  
 451 of folds in K-fold CV can affect bias and variance; thus, experimenting with different numbers of folds, especially  
 452 in smaller sample sizes, can be beneficial. Ultimately, the selection of appropriate evaluation techniques should be  
 453 tailored to the specific context of the dataset and the objectives of the modeling exercise, ensuring a robust and reliable  
 454 assessment of model performance.

### 455 3.2 Study 2: Misuse of Model Selection Can Lead to Over-Optimistic Performance Estimates

456 The evaluation bias was visualized using box plots (Figure 5), with the feature selection factor (FS) on the x-axis and  
 457 hyperparameter tuning (HT) distinguished by color — green for incorrect and yellow for correct implementation. The y-  
 458 axis represents the evaluation bias as measured by the correlation coefficient. The results indicate a clear overestimation  
 459 of model performance when feature selection is applied to the entire dataset, regardless of hyperparameter tuning. The  
 460 median biases were 0.797 for “FS=0; HT=0” and 0.761 for “FS=0; HT=1”. Moreover, inappropriate evaluation in  
 461 hyperparameter tuning resulted in a significant bias ( $p$ -value  $< 0.001$ ) with a median of 0.113 for “FS=1; HT=0”. The  
 462 only scenario without bias significantly occurred when both feature selection and hyperparameter tuning were correctly  
 463 incorporated within the cross-validation process “FS=1; HT=1”, yielding a median bias of -0.008. These findings align

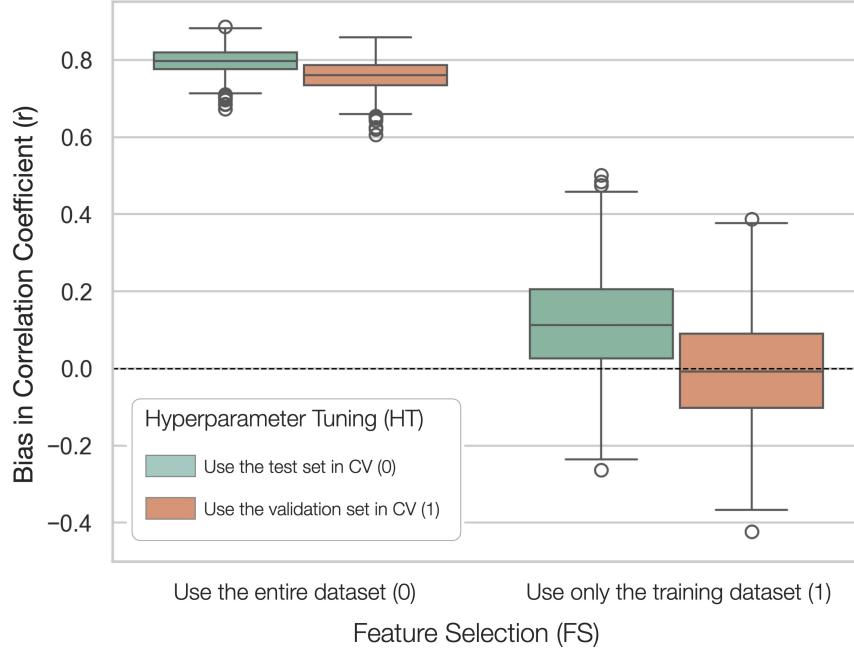


Figure 5: The evaluation bias of the four model selection strategies.

464 with the initial hypothesis and the prevailing literature, reinforcing that model selection must be integrated into the  
 465 cross-validation workflow to prevent an overestimation of model performance.

466 The simulation results robustly confirm the hypothesis that improper implementation of model selection inflates  
 467 performance estimates. Specifically, the evaluation bias is markedly high when feature selection precedes data splitting,  
 468 with or without correct hyperparameter tuning. Although integrating feature selection within cross-validation folds  
 469 mitigates this bias, incorrect hyperparameter tuning still significantly skews performance metrics. Notably, this  
 470 overestimation from the hyperparameter tuning is even more pronounced in complex models, such as neural network  
 471 architectures that often entail over a million parameters. These findings underscore the necessity of meticulous cross-  
 472 validation practices, particularly for feature selection and hyperparameter tuning, to ensure accurate performance  
 473 estimations and generalizability in predictive modeling.

### 474 3.3 Study 3: Overlooking Experimental Block Effects Can Lead to Biased Model Performance Estimates

475 In this simulation, an ANOVA table (Table 3), calculated from a single iteration for illustrative purposes, demonstrates  
 476 that the simulated data exhibits block variation significantly greater than the residual variance. The result (Figure 6)  
 477 shows that regardless of the amplitude of block effects in this simulation study, the Block CV strategy consistently yields  
 478 a mean performance estimate close to zero, while the Random CV strategy consistently and significantly overestimates  
 479 the model performance ( $p$ -value  $< 0.001$ ). This finding supports the hypothesis that Random CV tends to overestimate  
 480 model performance when block variation predominates over residual variation.

Table 3: ANOVA results for a single iteration of the simulated data with  $b = 0.5$ . SS: sum of squares; DF: degree of freedom; MS: mean square; F: F-statistic

| Source  | SS     | DF | MS     | F      | p-value |
|---------|--------|----|--------|--------|---------|
| Between | 60.971 | 4  | 15.243 | 20.580 | <0.001  |
| Within  | 70.363 | 95 | 0.741  |        |         |
| Total   | 131.35 | 99 |        |        |         |

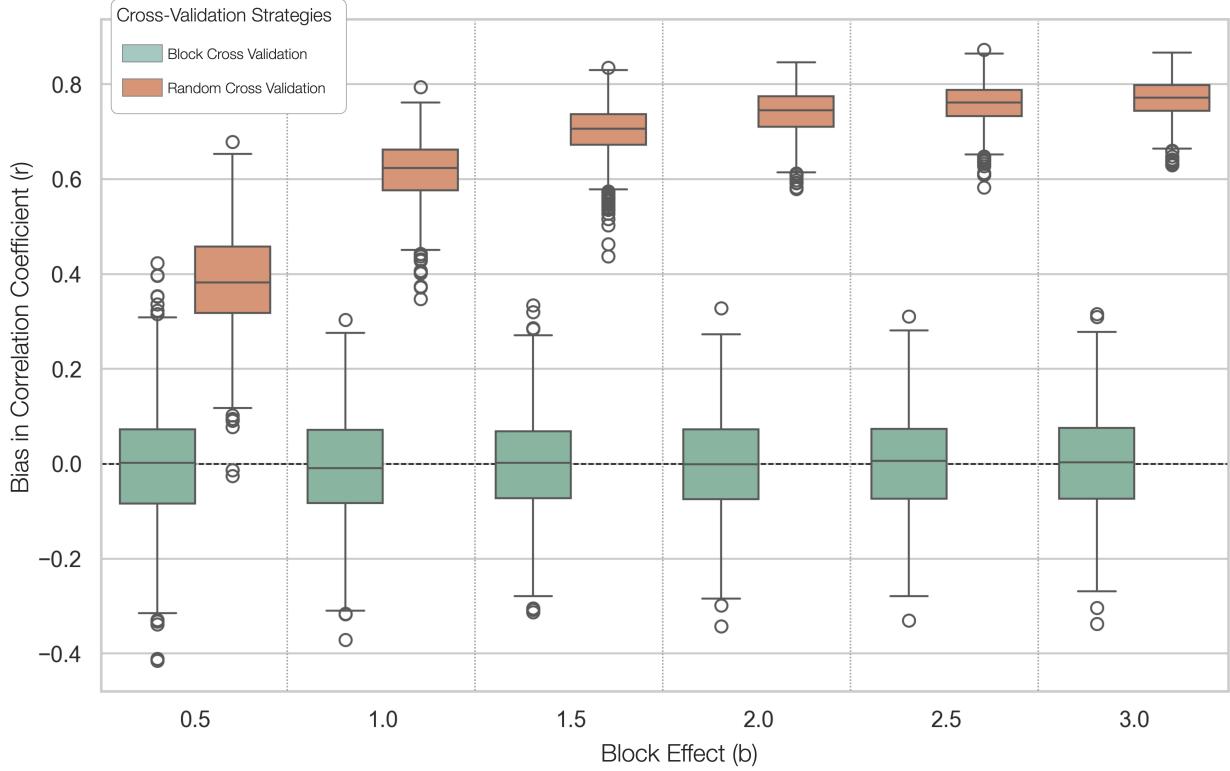


Figure 6: Bias in model performance estimation by Block CV and Random CV across 1000 iterations. The dashed line represents the null hypothesis that the mean performance estimate is zero.

481 In conclusion, block CV proves to be a vital tool in assessing the generalizability and accuracy of a predictive model,  
 482 especially in contexts where block effects, such as herd variations, play a significant role in both the predicting features  
 483 and response variable. The random CV strategy, which randomly assigns samples to folds without considering block  
 484 effects, tends to overestimate model performance. This study recommends that block CV be used as a benchmark in  
 485 model evaluation, especially when block effects are present

#### 486 3.4 Study 4: Different Regression Metrics Illustrate Different Aspects of Model Performance

487 The simulated hypothetical example in Figure 7 illustrates the performance of four different prediction scenarios. The  
 488 error-based metrics, RMSE and RMSPE, are sensitive to the magnitude of the error. In Scenario "Scaled", where the  
 489 errors are five times larger but remain the same in rank order compared to Scenario "Baseline", the RMSE inflates from

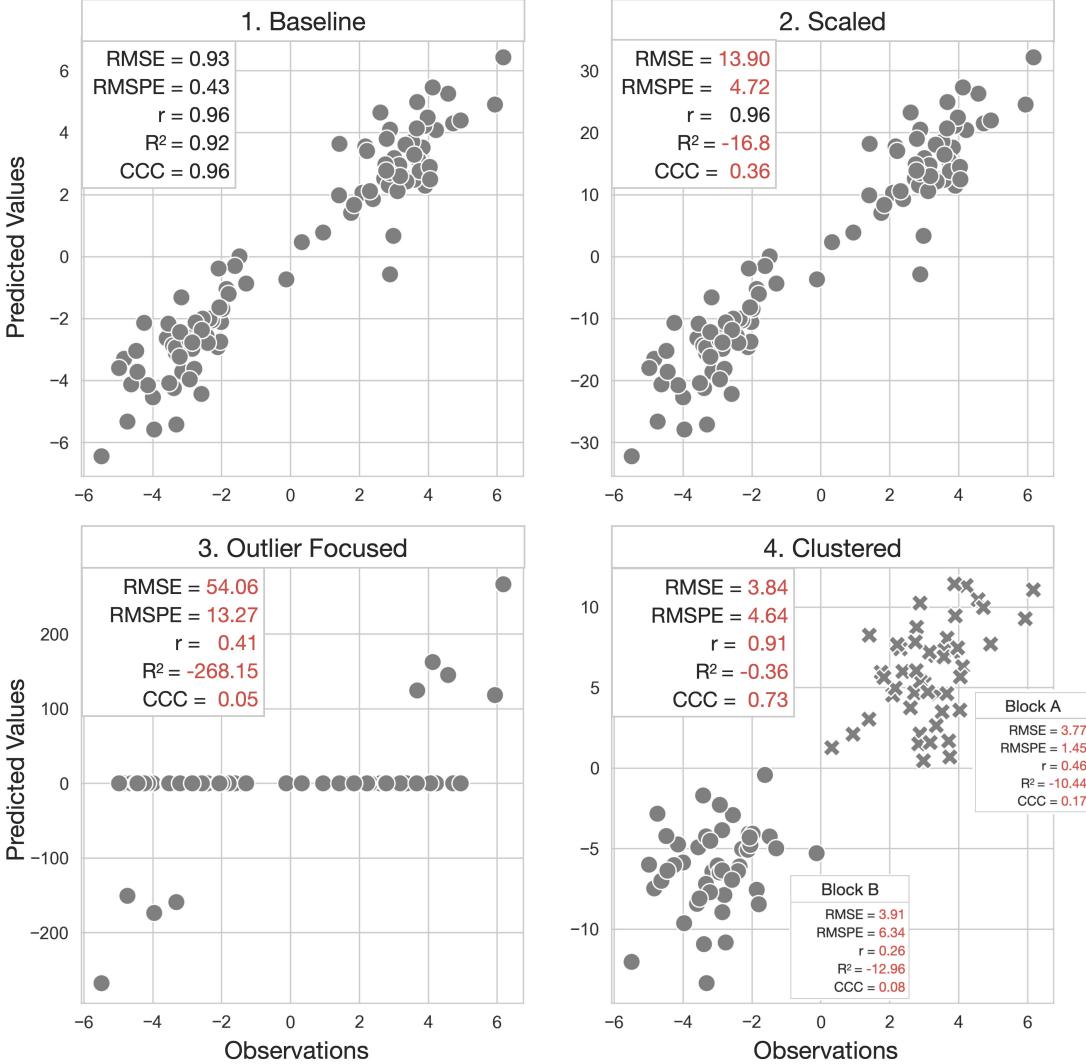


Figure 7: Scatter plots display the same observations against four different prediction scenarios in the given hypothetical example. Scenario "Baseline" serves as a baseline for the metrics, with any metric better than the baseline highlighted in bold and underscored, and any worse metric colored in red.

490 0.93 to 13.90, and RMSPE also increases from 0.43 to 4.72. Another notable characteristic of RMSE and RMSPE is  
 491 that they weigh more on large errors, which is essential when making a large error is costly and should be prioritized  
 492 for avoidance. In Scenario "Outliers", where certain predictions deviate substantially from the majority, the squaring  
 493 operation in Equation 1 accentuates these outliers, culminating in an RMSE of 54.06 and RMSPE of 13.27. However,  
 494 when investigating into the intra-block performance in the scenario "Clustered", the RMSE failed to detect the inflated  
 495 performance due to the strong block effects. It resulted in a similar RMSE of 3.84 from the entire prediction set and  
 496 3.77 and 3.91 within each block. This phenomenon emphasizes again that RMSE is affected solely by the magnitude  
 497 of the error, which neglects the ability of the model to capture relative trends in intra-block or inter-block predictions.  
 498 On the other hand, when the goal is to rank observations of interest rather than predict the absolute magnitude of the  
 499 error, linearity-based metrics can provide more insights. The correlation  $r$  is an example showing its consistency across

500 the Scenario "Baseline" and "Scaled", despite the latter having five times larger errors. This metric is particularly  
501 useful when the relative order of predictions is more important than the absolute error magnitude. However, it is  
502 worth noting that the correlation  $r$  can be misleading in certain scenarios, such as the Scenario "Outlier Focused",  
503 where 90% of the predictions are zero. In this case, the correlation  $r$  show a moderate performance of 0.41, which is  
504 mainly contributed by the 10% of the outlier predictions that are "ranked" correctly but with a large error magnitude.  
505 This example highlights the importance of visually inspecting the regression results through scatter plots to avoid  
506 misleading conclusions. Moreover, one common pitfall of the correlation  $r$  is that block effects can influence it, leading  
507 to an inflated performance estimate if individual variation is of greater interest than inter-block variation. This was  
508 demonstrated in Scenario "Clustered", where the overall coefficient  $r$  was 0.91, but the metric within each block was  
509 only 0.46 and 0.26, respectively. Therefore, it is essential to examine regression results within identifiable blocks.  
510 Besides the correlation  $r$ ,  $R^2$  provides a more comprehensive insight, as it focuses both the linear trend from the variance  
511 composition and the error magnitude from the residual sum of squares. From the "Scaled" scenario,  $R^2$  successfully  
512 detected the inflated error magnitude, resulting in a negative value of -16.8. It also captured the outlier-induced variance  
513 in the "Outliers" scenario, with a negative value of -268.15. Lastly, in Scenario "Clustered", the value of  $R^2$  indicated a  
514 weak performance by the model with a score of -0.36. This score is statistically reasonable, as the predictions have  
515 larger variance than the observations. The metric also successfully detected the model failure in capturing intra-block  
516 variation, as the  $R^2$  values within each block were -10.44 and -12.96, respectively. However, an obvious limitation  
517 of  $R^2$  is that it has no standard scale. Considering this, a more nuanced evaluation metric,  $CCC$ , showcases a more  
518 balanced performance evaluation. It always range from -1 to 1, and it successfully captures all the characteristics of the  
519 four scenarios. In Scenario "Scaled", the  $CCC$  value dropped from 0.96 to 0.36. In Scenario "Outliers", the  $CCC$   
520 value plummeted to 0.05, showcasing the model's failure to "align" the predictions with the observations with 90% of  
521 the predictions being zero. In the Scenario "Clustered", although the  $CCC$  value was 0.73, the metric also showed  
522 the model's weakness in each block, with the  $CCC$  values of 0.17 and 0.08, respectively. This study demonstrates  
523 that  $CCC$  is a more balanced metric that considers both the linear trend and the error magnitude, making it a more  
524 comprehensive evaluation metric for regression models.

### 525 3.5 Study 5: Label-Invariant Metrics Provide Balanced Assessment in Binary Classification

526 Different metrics in binary classification were evaluated in a simulated example (Figure 8). The original labels were  
527 inverted to examine the robustness of the metrics against label choices. The accuracy metric, with a 0.5 threshold in  
528 this example, stands at 0.60. This figure might suggest modest efficacy, marginally surpassing random chance, with an  
529 accuracy of 0.50. Nonetheless, the same accuracy level could be achieved by classifying every sample as negative in an  
530 imbalanced dataset where negatives are predominant. In contrast, precision and recall provide a more nuanced evaluation  
531 of model performance by separately assessing the correctness of positive predictions and the ability to detect actual  
532 positives. With a threshold of 0.5, the example dataset yields precision and recall values of 0.5 and 0.25, respectively.  
533 These metrics deliver more interpretable information that only half of the positive predictions are correct, and just a

| Ground Truth and Prediction Probability |  | Original Labels |                        | Inverted Labels |                        |
|---|--|-----------------|------------------------|-----------------|------------------------|
| ID                                      |  | Ground Truth    | Prediction Probability | Ground Truth    | Prediction Probability |
| 1                                       |  | (+)             | 0.99                   | (-)             | 0.01                   |
| 2                                       |  | (-)             | 0.70                   | (+)             | 0.30                   |
| 3                                       |  | (+)             | 0.38                   | (-)             | 0.62                   |
| 4                                       |  | (+)             | 0.33                   | (-)             | 0.67                   |
| 5                                       |  | (+)             | 0.26                   | (-)             | 0.74                   |
| 6                                       |  | (-)             | 0.16                   | (+)             | 0.84                   |
| 7                                       |  | (-)             | 0.15                   | (+)             | 0.85                   |
| 8                                       |  | (-)             | 0.14                   | (+)             | 0.86                   |
| 9                                       |  | (-)             | 0.12                   | (+)             | 0.88                   |
| 10                                      |  | (-)             | 0.07                   | (+)             | 0.93                   |

| Confusion Matrixes                |             | Original Labels @0.50   | Inverted Labels @0.50                           |  |     |     |     |
|-----------------------------------|-------------|---|---|--|-----|-----|-----|
| Ground Truth                      | Predictions | (+)   | (-)   | (+)  | (-) | (+) | (-) |
| (+)                               | TP          | FN  | → Recall or Sensitivity<br>$\frac{TP}{TP + FN}$ | 1  | 3   | 5   | 1   |
| (-)                               | FP          | TN  | → Specificity<br>$\frac{FP}{FP + TN}$           | 1  | 5   | 3   | 1   |
| Precision<br>$\frac{TP}{TP + FP}$ |             | Accuracy@0.50 = 0.600<br>Precision@0.50 = 0.500<br>Recall@0.50 = 0.250<br>MCC@0.50 = 0.100<br>PR AUC = 0.767<br>ROC AUC = 0.875 |   | Accuracy@0.50 = 0.600<br>Precision@0.50 = <u>0.625</u><br>Recall@0.50 = <u>0.833</u><br>MCC@0.50 = 0.100<br>PR AUC = <u>0.941</u><br>ROC AUC = 0.875 |     |     |     |

Figure 8: Simulated hypothetical example of binary classification. TP: true positive; FN: false negative; FP: false positive; TN: true negative; **Upper:** The ground truth and prediction probability. **Lower:** The confusion matrix of the prediction at a threshold of 0.5, followed by classification metrics of accuracy, precision, recall, MCC, PR curve AUC, and ROC curve AUC. The performance of the original labels serves as a baseline for comparison. Any better performance metrics from the inverted labels are highlighted in bold and underscored

quarter of the actual positives are detected. This contrasts with an accuracy of 0.6, which may appear misleadingly high due to the abundance of negative samples. Additionally, it is noted that the chosen confidence threshold significantly impacts precision and recall. While the trade-off between these two metrics is not always linear, it is generally observed that a higher threshold increases precision but decreases recall, and vice versa. A high threshold indicates a conservative approach in predicting positives, reducing false positives, and thus enhancing precision. However, this often leads to missing actual positive cases, lowering recall. Hence, the Precision-Recall (PR) curve is an essential tool for evaluating model performance across various thresholds. Plotted with recall on the x-axis and precision on the y-axis, this curve is derived by computing these metrics at different thresholds (Figure 9, Left). The Area Under the Curve (AUC) provides a summary measure of the PR curve's overall performance. A model's effectiveness is generally indicated by how close

543 a point on the PR curve is to the top-right corner. For example, at a threshold of 0.25, which is positioned near the  
 544 top-right of the PR curve, the model demonstrates impressive performance with an accuracy of 0.90, precision of 0.80,  
 545 and recall at 1.00.

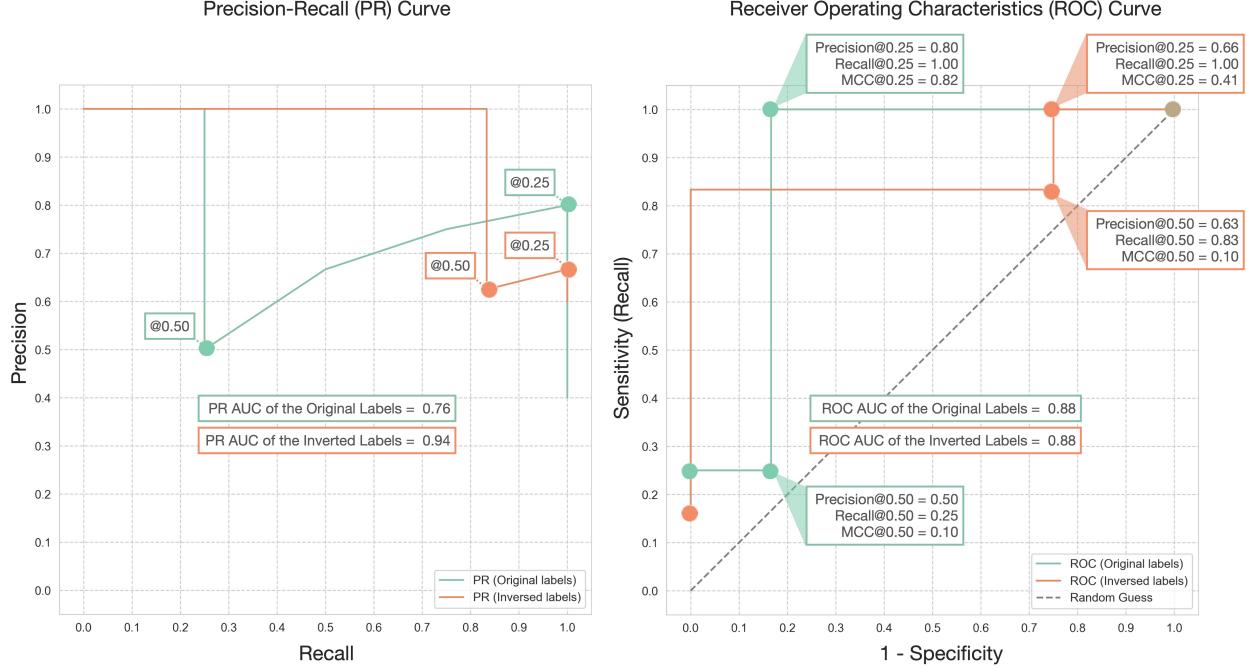


Figure 9: (**Left**) Precision-recall (PR) curve and (**Right**) Receiver operating characteristic (ROC) curve for the hypothetical example are displayed. The performance at confidence thresholds of 0.25 and 0.50 is highlighted. Original labels are marked in green, while inverted labels appear in orange. The Area Under the Curve (AUC) is depicted at the center of each curve.

546 However, it is worth re-emphasizing that precision and recall focus predominantly on positive samples. Inappropriately  
 547 assigning a predominant background event as the positive class can lead to skewed interpretations. This pitfall is  
 548 demonstrated in this example by inverting the labels. At a threshold of 0.50, precision increases from 0.50 to 0.63, and  
 549 recall jumps from 0.25 to 0.83. With the threshold set at 0.25, precision drops to 0.66 from 0.80, while recall remains  
 550 unchanged. The PR AUC also rises from 0.76 to 0.94. Such shifts in metrics, driven merely by label rearrangement  
 551 unrelated to the data or model characteristics, underscore the importance of label-invariant metrics that remain unaffected  
 552 by label assignments. Unlike metrics focusing solely on positive samples, the ROC curve accounts for both positive  
 553 and negative samples, making it a label-invariant metric. Specificity is plotted on the x-axis and sensitivity on the  
 554 y-axis, calculated at different thresholds (Figure 9, Right). In this hypothetical example, the ROC curve demonstrates  
 555 robustness and label-invariance with a consistent AUC of 0.875, regardless of whether the original or inverted labels are  
 556 used. Lastly, another label-invariant metric is MCC which provides a balanced assessment of both positive and negative  
 557 samples. Considering MCC's balanced approach to evaluating model performance, this study introduces the concept  
 558 of an MCC curve. This curve, which plots the MCC value against various threshold levels (Figure 10), serves as a  
 559 powerful tool for identifying the optimal confidence thresholds for model predictions. By examining this curve, one

560 can determine the specific threshold at which the MCC value peaks, thereby optimizing the model's performance. For  
 561 example, when applied to the hypothetical example, the optimum MCC value of 0.82 was attained at a threshold of 0.25.  
 562 This particular threshold corresponded to accuracy, precision, and recall values of 0.90, 0.75, and 1.00, respectively.  
 563 Notably, the MCC curve retains its symmetry even when labels are reversed, affirming its status as a label-invariant  
 564 measure. In scenarios with inverted labels, the maximum MCC value observed was 0.83, achieved at a threshold of  
 565 0.75, leading to accuracy, precision, and recall values of 0.90, 1.00, and 0.83, respectively. Such findings underscore the  
 566 MCC's ability to provide a balanced and comprehensive assessment of both positive and negative samples, thereby  
 567 reinforcing its utility as a versatile and effective metric for thorough model evaluation.

568 In conclusion, binary classification models are often evaluated using metrics focusing on positive samples, such as  
 569 precision and recall. It is generally advisable to designate the event of interest as the positive class. Otherwise, these  
 570 metrics can be misleading when the more common but less significant background event is mistakenly marked as the  
 571 positive class. To circumvent this potential bias, adopting label-invariant metrics is recommended. These metrics offer  
 572 a more balanced and reliable assessment of model performance. Notable examples of such metrics include the ROC  
 573 curve and the proposed MCC curve by this review, both of which are unaffected by the choice of positive and negative  
 class labels and are thus robust for a thorough model evaluation.

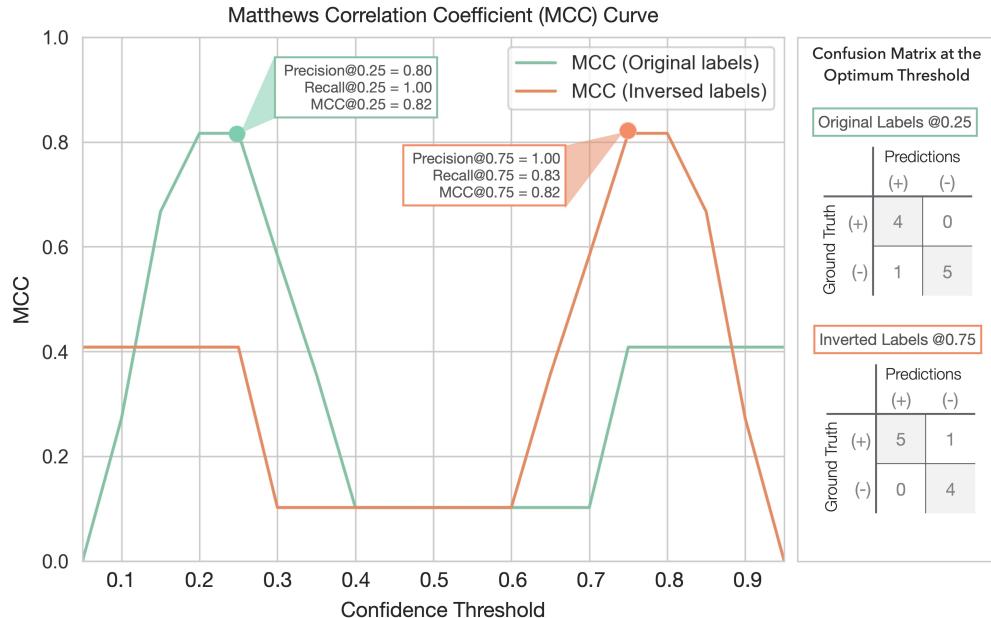


Figure 10: Matthews Correlation Coefficient (MCC) curve. A line chart plotting MCC at different thresholds for the hypothetical example. The optimal threshold is highlighted by the dot marks in green and orange for the original and inverted labels, respectively. The confusion matrix at the optimal threshold is displayed in the right panel.

**575 4 Conclusion**

576 In summary, the review highlights several key considerations for performance assessment in predictive modeling.  
577 When evaluating regression models, the choice of metrics like Correlation Coefficient  $r$ , RMSE, and  $R^2$  depends on  
578 the specific goals of the model. A comprehensive evaluation should include multiple metrics to understand different  
579 aspects of model performance. In binary classification models, precision and recall are crucial, but it is essential to  
580 correctly designate the positive class to avoid bias. Label-invariant metrics, such as the ROC curve and the proposed  
581 MCC curve, provide a balanced assessment, unaffected by class label choices. Additionally, the reliability of model  
582 evaluation is significantly influenced by estimator choice and sample size. Larger sample sizes tend to reduce bias and  
583 variance, increasing evaluation reliability. Cross-validation methods, such as K-fold CV and LOOCV, are preferable  
584 for unbiased performance estimation, with the number of folds in K-fold CV being particularly influential in smaller  
585 datasets. Moreover, the review underscores the importance of correct implementation in model selection processes,  
586 as improper techniques can inflate performance estimates. This is especially true in complex models where feature  
587 selection and hyperparameter tuning need meticulous cross-validation to avoid overestimation of performance. Finally,  
588 the utility of Block CV is emphasized in contexts where block effects are significant. It provides a more realistic  
589 assessment of model generalizability and accuracy compared to a Random CV, which tends to overestimate performance  
590 in such scenarios. Overall, the review recommends a thoughtful selection of metrics and evaluation techniques, tailored  
591 to the specific dataset and modeling objectives, to ensure accurate and reliable performance assessments in predictive  
592 modeling.

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706 **Appendix**

707 **Cross Validation**

708 Model cross validation aims to evaluate how well a given model generalizes to an independent dataset that it has not  
 709 seen during the training process. The most common method is K-fold cross-validation (**K-fold CV**). To implement the  
 710 K-fold CV, the available dataset, denoted as  $\mathcal{D}$ , is partitioned into K equally sized folds. We can express the dataset as  
 711 below:

$$\begin{aligned}\mathcal{D} &= \{(X, Y)\} \\ &= \{(X_1, Y_1), (X_2, Y_2), \dots, (X_K, Y_K)\}\end{aligned}\tag{17}$$

712 where  $X \in \mathbb{R}^{n \times p}$  represents the input features, and  $Y \in \mathbb{R}^{n \times 1}$  symbolizes the ground truth labels for a single target  
 713 variable. The value of n corresponds to the total number of samples, while p represents the number of features. In  
 714 each iteration of the K-fold CV, a single fold is reserved as the test set,  $\mathcal{D}_{\text{test}}$  (or  $\mathcal{D}_k$ ), to act as unseen data, while the  
 715 remaining folds make up the training set  $\mathcal{D}_{\text{train}}$  (or  $\mathcal{D}_{-k}$ ):

$$\begin{aligned}\mathcal{D}_{\text{train}} &= \mathcal{D}_{-k} \\ &= \{(X_1, Y_1), (X_2, Y_2), \dots, (X_{k-1}, Y_{k-1}), (X_{k+1}, Y_{k+1}), \dots, (X_K, Y_K)\} \\ \mathcal{D}_{\text{test}} &= \mathcal{D}_k \\ &= \{(X_k, Y_k)\}\end{aligned}\tag{18}$$

716 After splitting the dataset into  $\mathcal{D}_{-k}$  and  $\mathcal{D}_k$ , the examined model  $f$  is trained on the training set  $\mathcal{D}_{-k}$  and denoted as  $f_{\mathcal{D}_{-k}}$ .  
 717 The hold-out test set  $\mathcal{D}_k$  is then used to evaluate the model performance  $\hat{g}(f_{\mathcal{D}_{-k}})$ , which is defined by comparing the  
 718 predicted labels  $\hat{Y}_k = f_{\mathcal{D}_{-k}}(X_k)$  with the true labels  $Y_k$  using a performance metric  $\mathcal{L}$  (e.g., RMSE or  $R^2$ ):

$$\begin{aligned}\hat{g}(f_{\mathcal{D}_{-k}}) &= \mathcal{L}(Y_k, \hat{Y}_k) \\ &= \mathcal{L}(Y_k, f_{\mathcal{D}_{-k}}(X_k))\end{aligned}\tag{19}$$

719 To estimate the generalization performance of a model  $\mathbb{E}[\hat{g}(f_{\mathcal{D}})]$ , the K-fold CV procedure is repeated K times until  
 720 each fold has been used as the test set  $\mathcal{D}_k$  once. The entire dataset  $\mathcal{D}$  is leveraged to calculate the average prediction  
 721 performance over all K folds. The model's generalization performance can be expressed as:

$$\begin{aligned}\mathbb{E}[\hat{g}(f_{\mathcal{D}})] &= \mathbb{E}[\hat{g}(f_{\mathcal{D}_k})] \\ &= \frac{1}{K} \sum_{k=1}^K \hat{g}(f_{\mathcal{D}_k})\end{aligned}\tag{20}$$

722 It is noted that  $\mathbb{E}[\hat{g}(f_{\mathcal{D}})]$  is equivalent to  $\mathbb{E}[\hat{g}(f_{\mathcal{D}_k})]$  in K-fold CV. It is because the  $\mathbb{E}[\hat{g}(f_{\mathcal{D}})]$  is estimated by averaging  
 723 all  $\hat{g}(f_{\mathcal{D}_k})$  over K folds, which is also the definition of  $\mathbb{E}[\hat{g}(f_{\mathcal{D}_k})]$ .

#### 724 Cross Validation Bias and Variance

725 The true generalization performance of the model  $G(f_{\mathcal{D}})$  can only be approximated by averaging the performance  
 726 metrics over infinite unseen datasets. However, in practice, the dataset  $\mathcal{D}$  is finite and therefore, there is always a bias  
 727 when using a finite dataset to estimate  $G(f_{\mathcal{D}})$ . The bias is known as validation bias:

$$\text{Bias} = \mathbb{E}[\hat{g}(f_{\mathcal{D}})] - G(f_{\mathcal{D}})\tag{21}$$

728 For example, if RMSE is used as the performance metric, a positive validation bias suggests that the model validation  
 729 procedure concludes a pessimistic estimation of the model performance, since the true performance is expected to be  
 730 lower than the estimated performance. Another aspect of model validation is the variance of the estimated performance.  
 731 For example, in a 5-fold cross-validation, there are five estimates of the model performance. The variance among these  
 732 five estimates is known as validation variance. A high validation variance suggests that the performance is sensitive to  
 733 the choice of the test set  $\mathcal{D}_k$ , which may be caused by a small sample size or an over-complex model. The validation  
 734 variance can be defined as:

$$\begin{aligned}\text{Variance} &= \mathbb{E}[(\hat{g}(f_{\mathcal{D}_k}) - \mathbb{E}[\hat{g}(f_{\mathcal{D}})])^2] \\ &= \mathbb{E}[\hat{g}^2(f_{\mathcal{D}_k}) - 2\hat{g}(f_{\mathcal{D}_k})\mathbb{E}[\hat{g}(f_{\mathcal{D}})] + \mathbb{E}^2[\hat{g}(f_{\mathcal{D}})]] \\ &= \mathbb{E}[\hat{g}^2(f_{\mathcal{D}_k})] - 2\mathbb{E}[\hat{g}(f_{\mathcal{D}_k})]\mathbb{E}[\hat{g}(f_{\mathcal{D}})] + \mathbb{E}^2[\hat{g}(f_{\mathcal{D}})] \\ &= \mathbb{E}[\hat{g}^2(f_{\mathcal{D}_k})] - \mathbb{E}^2[\hat{g}(f_{\mathcal{D}})]\end{aligned}\tag{22}$$

735 Combining the Equations 21 and 22, the mean squared error (MSE) of the model validation can be decomposed as:

$$\begin{aligned}
\text{MSE} &= \mathbb{E}[(\hat{g}(f_{D_k}) - G(f_D))^2] \\
&= \mathbb{E}[\hat{g}^2(f_{D_k})] - 2\mathbb{E}[\hat{g}(f_{D_k})]G(f_D) + G^2(f_D) + \\
&\quad \mathbb{E}^2[\hat{g}(f_{D_k})] - \mathbb{E}^2[\hat{g}(f_{D_k})] \\
&= (\mathbb{E}^2[\hat{g}(f_{D_k})] - 2\mathbb{E}[\hat{g}(f_{D_k})]G(f_D) + G^2(f_D)) + \\
&\quad (\mathbb{E}[\hat{g}^2(f_{D_k})] - \mathbb{E}^2[\hat{g}(f_{D_k})]) \\
&= (\mathbb{E}[\hat{g}(f_{D_k})] - G(f_D))^2 + (\mathbb{E}[\hat{g}^2(f_{D_k})] - \mathbb{E}^2[\hat{g}(f_{D_k})]) \\
&= (\mathbb{E}[\hat{g}(f_D)] - G(f_D))^2 + (\mathbb{E}[\hat{g}^2(f_D)] - \mathbb{E}^2[\hat{g}(f_D)]) \\
&= \text{Bias}^2 + \text{Variance}
\end{aligned} \tag{23}$$

736 **Hyperparameter**

737 Here are the loss functions for ordinary least squares (OLS), ridge regression, and LASSO regression, respectively:

$$\mathcal{L}_{\text{OLS}}(\beta) = \sum_{i=1}^n (y_i - x_i \beta)^2 \tag{24}$$

$$\mathcal{L}_{\text{ridge}}(\beta) = \sum_{i=1}^n (y_i - x_i \beta)^2 + \lambda \sum_{j=1}^p \beta_j^2 \tag{25}$$

$$\mathcal{L}_{\text{LASSO}}(\beta) = \sum_{i=1}^n (y_i - x_i \beta)^2 + \lambda \sum_{j=1}^p |\beta_j| \tag{26}$$

738 Where  $x_i$  and  $y_i$  represent the  $i$ th row of the design matrix  $X$  and the response vector  $Y$ , respectively. The term  $n$   
 739 denotes the sample size, and  $\beta$  is the coefficient vector. All three models aim to find the optimal  $\beta$  that minimizes their  
 740 respective loss function,  $\mathcal{L}$ . In the regularized models (i.e., ridge and LASSO regression), the vector length of  $\beta$  is  
 741 penalized in the loss function.

742 **Squared Correlation Coefficient  $r^2$  and Determination Coefficient  $R^2$**

743 The squared Pearson correlation coefficient,  $r^2$ , is not necessarily equivalent to the coefficient of determination,  $R^2$ .  
 744 This equivalence holds true specifically in the context of least squares regression when the same model and data are  
 745 used for both fitting and evaluation. However, this may not be the case when the model is assessed using new data.  
 746 To demonstrate the equivalence between  $r^2$  and  $R^2$  under these specific conditions, we begin by assuming that the  
 747 covariance between the predicted values  $\hat{Y}$  and the residuals  $\epsilon$  is zero:

$$\begin{aligned}
\text{cov}(Y, \hat{Y}) &= \text{cov}(\hat{Y} + \epsilon, \hat{Y}) \\
&= \text{cov}(\hat{Y}, \hat{Y}) + \text{cov}(\hat{Y}, \epsilon) \\
&= \text{var}(\hat{Y}) + \text{cov}(\hat{Y}, \epsilon) \\
&= \text{var}(\hat{Y})
\end{aligned} \tag{27}$$

748 With the assumption that  $\bar{\hat{Y}} = \bar{Y}$ , which typically holds when  $\mathbb{E}[\epsilon] = 0$ , the squared correlation coefficient  $r^2$  is  
 749 expressed as follows:

$$\begin{aligned}
r^2 &= \frac{\text{cov}^2(Y, \hat{Y})}{\text{var}(Y)\text{var}(\hat{Y})} \\
&= \frac{\text{var}(\hat{Y})^2}{\text{var}(Y)\text{var}(\hat{Y})} \\
&= \frac{\text{var}(\hat{Y})}{\text{var}(Y)} \\
&= \frac{\sum_{i=1}^n (\hat{Y}_i - \bar{\hat{Y}})^2}{\sum_{i=1}^n (Y_i - \bar{Y})^2} \\
&= \frac{\sum_{i=1}^n (\hat{Y}_i - \bar{\hat{Y}})^2}{\sum_{i=1}^n (Y_i - \bar{Y})^2} \\
&= \frac{SS_{\text{regression}}}{SS_{\text{total}}} \\
&= R^2
\end{aligned} \tag{28}$$

750 where  $SS_{\text{regression}}$  is the variation explained by the model and  $SS_{\text{total}}$  is the total sum of squares. Each  $Y_i$  and  $\hat{Y}_i$  are the  
 751  $i$ th elements of the actual response vector  $Y$  and the predicted response vector  $\hat{Y}$ , while  $\bar{Y}$  and  $\bar{\hat{Y}}$  are their respective  
 752 means. This proof highlights that under certain assumptions,  $r^2$  and  $R^2$  can indeed be equivalent, but such conditions  
 753 are specific to least squares regression where errors are normally distributed and predictions are unbiased estimates of  
 754 the actual values.