
COMMON PITFALLS IN EVALUATING MODEL PERFORMANCE AND STRATEGIES FOR AVOIDANCE

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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 Modeling**

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

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

40 **1.2 Model Evaluation**

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

48 The most common CV method is K-fold CV, which partitions the dataset into K equally sized folds. In each iteration,
49 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

50 (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
51 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
52 performance over all K folds is deemed as the expected generalization performance of the model $\mathbb{E}[\hat{g}]$ on new data.

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

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

71 Leave-one-out cross-validation (LOOCV) is a variant of K-fold CV where K equals the sample size of the complete
72 dataset \mathcal{D} . It provides an unbiased estimation of model performance because the training set $\mathcal{D}_{\text{train}}$ closely resembles the
73 unseen population of interest, given its size of $N - 1$, where N is the sample size. However, as the trade-off discussion
74 suggested, this method can lead to high validation variance due to the model being evaluated on one sample at a time.
75 The true unbiased nature of LOOCV is fully realized only when all K folds are utilized. Performing an incomplete
76 LOOCV can introduce significant bias because of the inherent high validation variance, which often occurs when
77 training each model iteration is prohibitively time-consuming or computationally demanding. In specific contexts, such
78 as genomic prediction, strategies like the one described by Cheng et al. leverage the matrix inverse lemma, which
79 allows for computational savings by avoiding the inversion of large matrices in each fold. This technique significantly
80 reduces the dependency of computational resources on the sample size (?). Van Dixhoorn et al. exemplify the use of
81 LOOCV with a small dataset, aiming to predict cow resilience with limited data resources (?). Nevertheless, for large
82 datasets, LOOCV is generally not recommended due to computational inefficiency. Further details of bias-variance
83 trade-off have been extensively explored in the statistical literature (??).

84 1.3 Model Selection

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

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

119 milk (?). Similarly, Becker et al. demonstrated a robust evaluation by using nested cross-validation loops; the inner
120 loop conducted a grid search for the best hyperparameters in logistic regression, while the outer loop was designed to
121 evaluate the performance of the resulting optimized model (?). Both examples underscore the importance of separating
122 model selection from performance evaluation to ensure the validity and reliability of the results.

123 **1.4 Cross Validation Design with Block Effects**

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

144 **1.5 Model Performance Metrics**

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

151 **1.5.1 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	$[-1, 1]$

152 Regression models aim to predict continuous variables and are commonly employed in diverse applications, such
 153 as estimating body condition scores (??), body weight (??), milk composition (????), efficiency of feed resource
 154 usage (??), and early-lactation behavior (?). The metrics in regression tasks evaluate the agreement between the
 155 predicted value \hat{y} and the true values y . The agreement can be generally quantified in two ways: error-based metrics
 156 and linearity-based metrics. The metrics are summarized in Table ??.

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

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

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

160 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
 161 of the original data, making them easy to interpret in real-world units. Additionally, compared to MAE, RMSE penalizes
 162 large errors more due to the squared term, making it more sensitive to outliers. In the cow production, monitoring
 163 animal body weight is a common practice to aid in the management of dairy cows. Studies by Song et al. and Xavier et
 164 al. have utilized RMSE to assess the effectiveness of three-dimensional cameras in estimating dairy cow body weight,
 165 yielding RMSE values of 41.2 kg and 12.1 kg, respectively (??). These figures provide a straightforward value for
 166 farmers to gauge whether the prediction error is tolerable, considering their specific operational costs and management
 167 thresholds. In essence, RMSE translates complex model accuracy into practical insights for productive agricultural
 168 units. When evaluating the same model across different traits, which may have different scales, a common practice is to
 169 express error metrics in a scale-free manner. This can be achieved by expressing RMSE as a percent of the deviation
 170 from the observed value, such as root mean squared percentage error (RMSPE), or as a Root Mean Standard Deviation
 171 Ratio (RSR) that normalizes the RMSE by the standard deviation of the observed values:

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

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

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

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

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

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

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

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

191 The coefficient of determination R^2 quantifies model performance from the proportion of variance in the dependent
 192 variable that is predictable from the independent variables. It ranges from negative infinity to 1, where 1 indicates
 193 that the model explains all the variance in the dependent variable, and 0 indicates that the model performs no better

194 than predicting all samples as the mean of the observed values. R^2 is useful in comparing multiple regression models,
 195 as demonstrated in studies that regress body weight of dairy cows on a set of morphological traits (?), examine
 196 the relationship between milk spectral profiles and nitrogen utilization efficiency (?), and evaluate the predictive
 197 performance of milk fatty acid composition (?).

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

205 In addition to r^2 and R^2 , another linearity-based metric is Lin's concordance correlation coefficient (CCC) (?):

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

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

213 1.5.2 Metrics in Classification Tasks

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

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

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

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

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

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

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

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

226 Precision and recall refine the assessment of a classification model by offering insights that accuracy alone may
 227 overlook. Precision calculates the fraction of true positives among all positive predictions, essentially measuring
 228 the trustworthiness of positive predictions made by the model (Eq. ??). High precision is crucial in scenarios where
 229 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 (?) or mastitis (?) 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. ??). 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 (?) and impact welfare-related transport decisions (?). An automated detection system (???) 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. ??). 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:

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

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

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 (?) and diagnosing pregnancy using spectroscopy technology (?). 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.

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

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

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

263 1.6 Study Objectives

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

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

282 **2 Materials and Methods**

283 **2.1 Study 1: Evaluation bias and variance of cross-validation**

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

297 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
 298 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
 299 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
 300 β , 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:

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

301 For the "In-Sample" performance estimator, predictions were made without splitting, as:

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

302 Where:

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

310 Estimated performance $\mathbb{E}[\hat{g}(f_{\mathcal{D}})]$ was derived by averaging the performance metrics across all K folds as per Eq. ??.

311 The bias and variance of the evaluation were calculated using Eqs. ?? and ??, respectively. To approximate true

312 model performance $G(f_{\mathcal{D}})$, a hundred unseen datasets \mathcal{D}^* were generated identically to \mathcal{D} , and the performance $G(f_{\mathcal{D}})$

313 was estimated by averaging the performance metrics across all \mathcal{D}^* . The detailed steps to compute evaluation bias and

314 variance are provided in the supplementary materials.

315 2.2 Study 2: Model Selection in Cross-Validation

316 The objective of this simulation study is to examine the effect of improper model selection implementation on validation

317 bias. The focus will be on the model selection procedures of feature selection and hyperparameter tuning. The study

318 hypothesizes that utilizing the test set inappropriately during any model selection stage will lead to a significant

319 overestimation of model performance. This study simulated a regression task using an SVR model, which utilized

320 various kernel functions to project a subset of features, X, to predict a target variable, Y. Both X and Y are drawn from

321 a normal distribution $\mathcal{N}(0, 1)$ to establish a baseline null correlation (performance r=0) for assessing validation bias.

322 This study set the sample size and number of features at 100 and 1000, respectively. Feature selection is executed by

323 choosing the top 50 features that correlate most strongly with Y. For hyperparameter tuning, four kernel functions were

324 evaluated: linear, polynomial, radial basis function, and sigmoid.

325 This study introduces notations FS for feature selection and HT for hyperparameter tuning, assigning a binary indicator

326 (0 or 1) to denote incorrect (0) or correct (1) implementation of model selection. This yields four possible combinations

327 of model selection strategies: “FS=0; HT=0”, “FS=0; HT=1”, “FS=1; HT=0”, “FS=1; HT=1” (Figure ??). When

328 FS=0, feature selection precedes cross-validation splitting. If FS=1, feature selection occurs within each fold of the

329 training set during cross-validation. With hyperparameter tuning, a correct implementation (HT=1) involves splitting

330 the dataset into training (64%), validation (16%), and test (20%) sets. The model is trained and tuned using the training

331 and validation sets, respectively, while the test set is reserved for a single evaluation of model performance. Conversely,

332 with HT=0, only training (80%) and test (20%) sets are used, risking validation bias as the test set informs both

333 training and performance reporting. A 5-fold cross-validation approach was deployed for all strategies. Validation

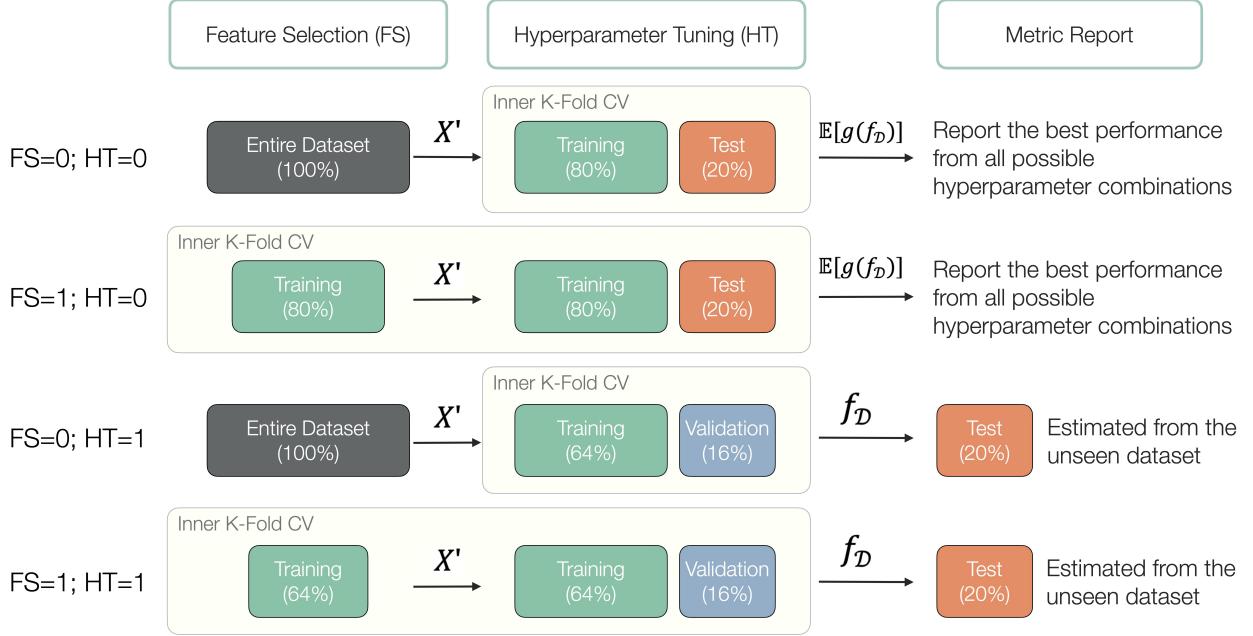


Figure 1: Workflow diagram illustrating four cross-validation strategies of feature selection (FS) and hyperparameter tuning (HT), where 0 denotes incorrect implementation and 1 indicates correct practice. X' is the selected feature subset, $\mathbb{E}[\hat{g}(f_D)]$ is the expected generalization performance,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

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

338 2.3 Study 3: Block Effects in Cross-Validation

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

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

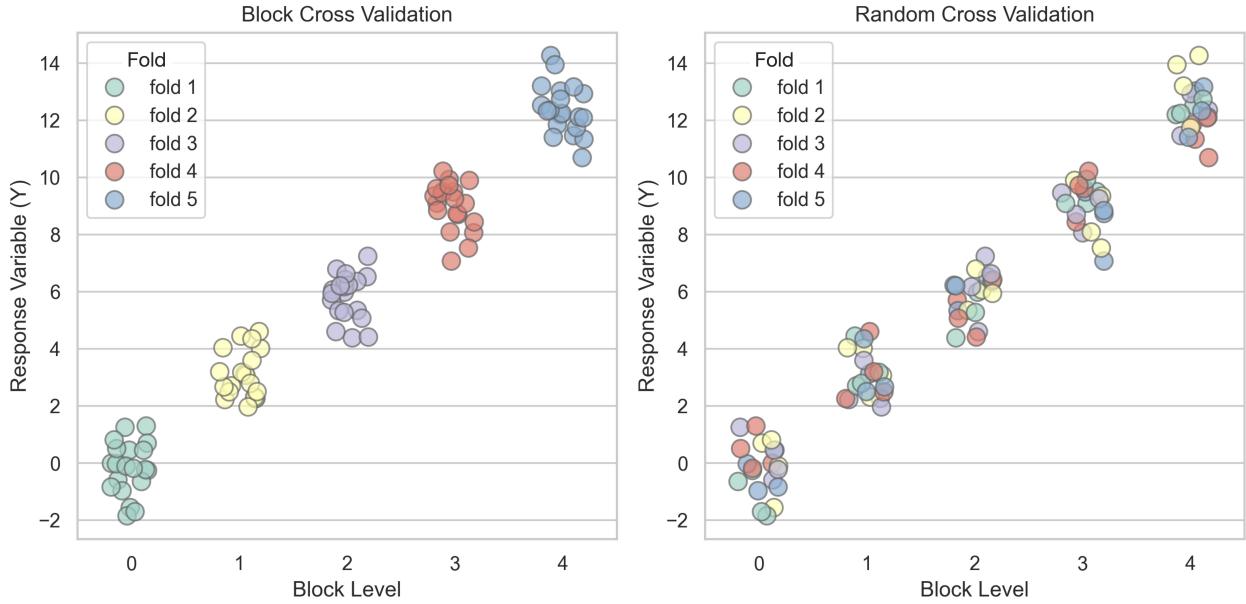


Figure 2: Illustration of fold assignment in block cross validation (left) and random cross validation (right). Folds are color-coded, and the block effect is set to 3 in this example.

356 2.4 Study 4: Performance Metrics in Regression Tasks

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

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

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

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

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

403 2.5 Study 5: Performance Metrics in Classification Tasks

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

425 **3 Results and Discussion**

426 **3.1 Study 1: The Impact of Estimator Choice and Sample Size on Model Evaluation Reliability**

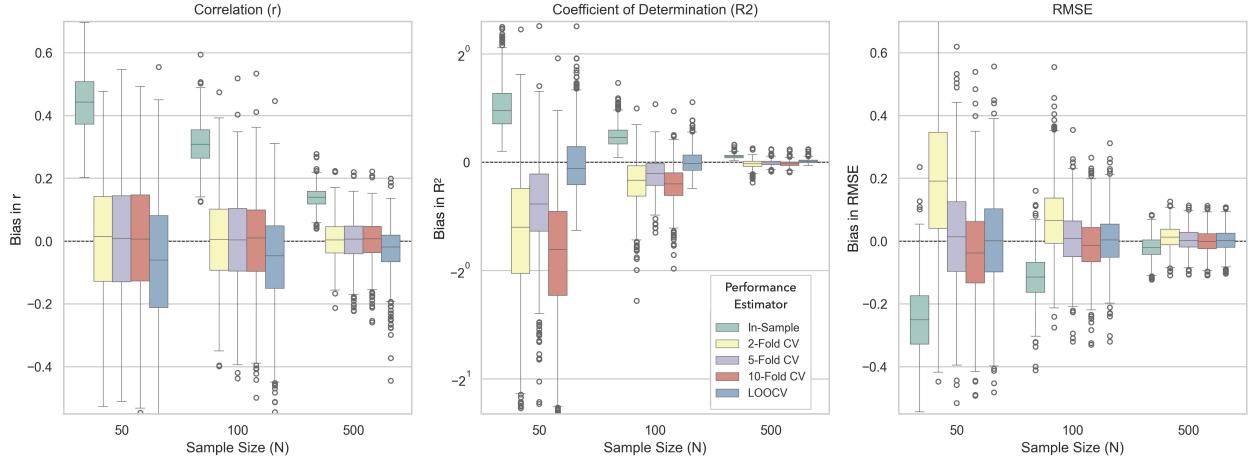


Figure 3: Simulation results of evaluation bias from 1000 sampling iterations. Multiple performance estimators across different sample sizes were color-coded. Three metrics: r , R^2 , and RMSE, were displayed in the column facets.

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

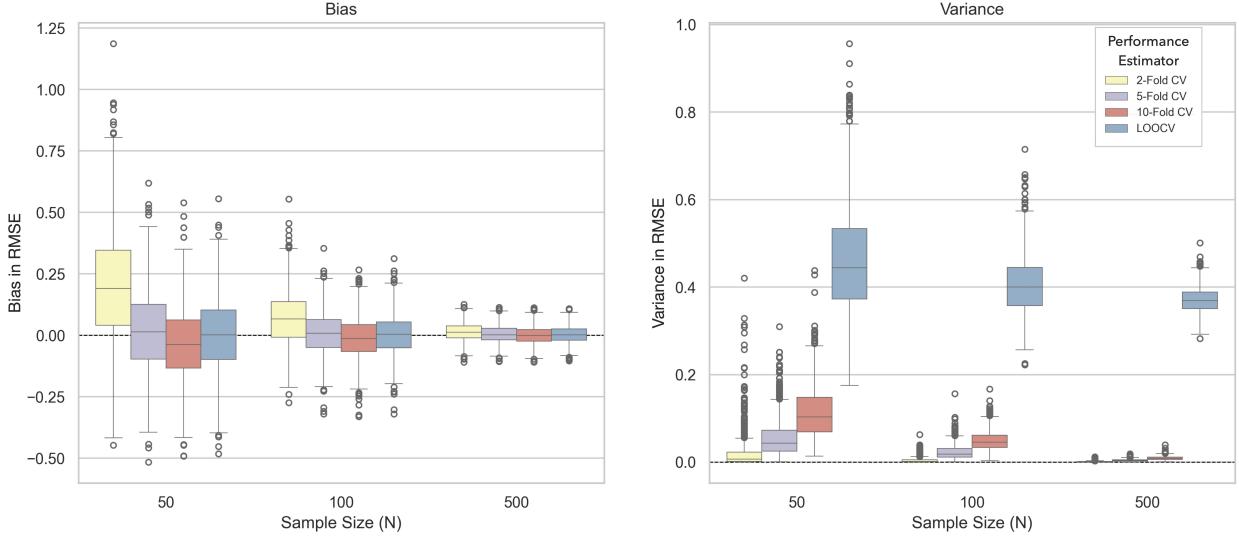


Figure 4: Simulation results of evaluation bias and variance from 1000 sampling iterations. Multiple performance estimators across different sample sizes were color-coded. Only RMSE was displayed. Bias and variance were listed in the left and right facets, respectively.

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

454 3.2 Study 2: Misuse of Model Selection Can Lead to Over-Optimistic Performance Estimates

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

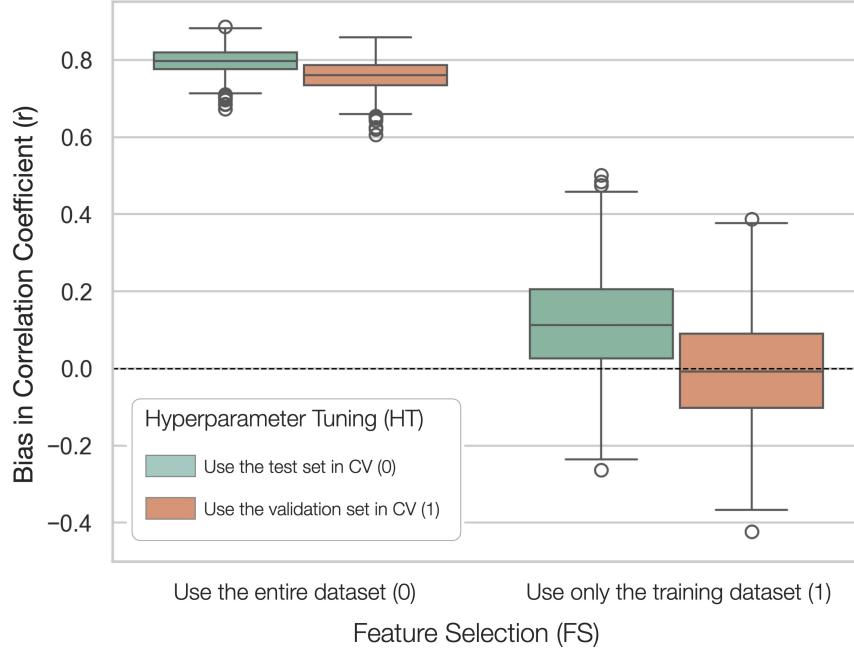


Figure 5: The evaluation bias of the four model selection strategies.

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

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

473 3.3 Study 3: Overlooking Experimental Block Effects Can Lead to Biased Model Performance Estimates

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

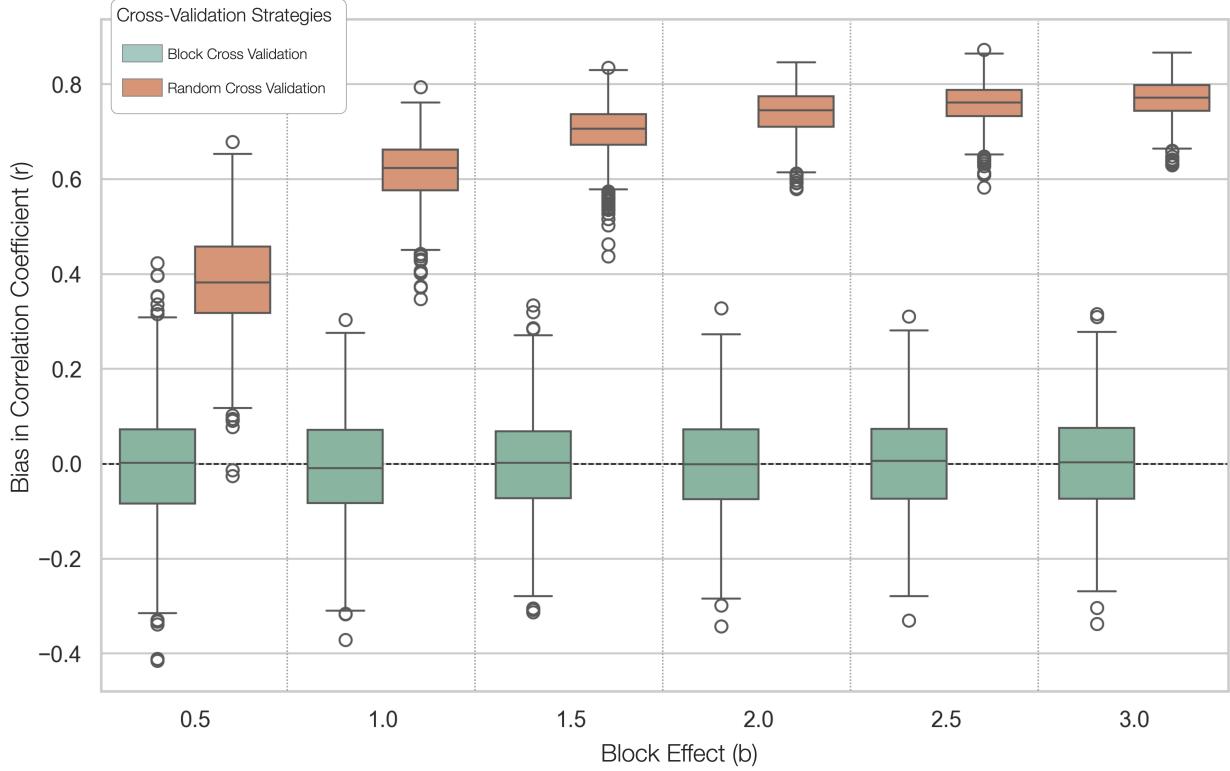


Figure 6: Bias in model performance estimation by Block CV and Random CV across 1000 iterations. The dashed line represents the null hypothesis that the mean performance estimate is zero.

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

485 3.4 Study 4: Different Regression Metrics Illustrate Different Aspects of Model Performance

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

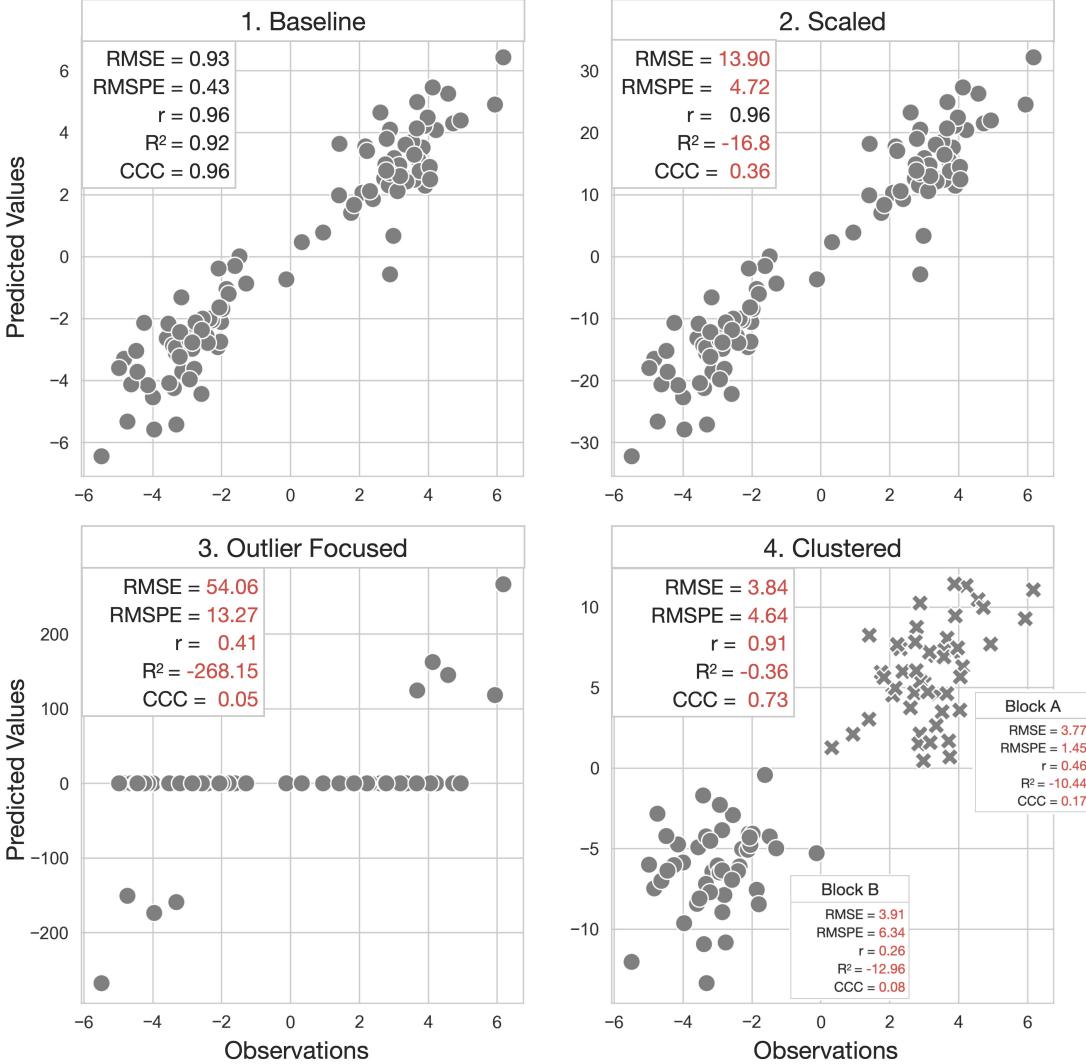


Figure 7: Scatter plots display the same observations against four different prediction scenarios in the given hypothetical example. Scenario "Baseline" serves as a baseline for the metrics, with any metric better than the baseline highlighted in bold and underscored, and any worse metric colored in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

489 0.93 to 13.90, and RMSPE also increases from 0.43 to 4.72. Another notable characteristic of RMSE and RMSPE is
 490 that they weigh more on large errors, which is essential when making a large error is costly and should be prioritized
 491 for avoidance. In Scenario "Outliers", where certain predictions deviate substantially from the majority, the squaring
 492 operation in Equation ?? accentuates these outliers, culminating in an RMSE of 54.06 and RMSPE of 13.27. However,
 493 when investigating into the intra-block performance in the scenario "Clustered", the RMSE failed to detect the inflated
 494 performance due to the strong block effects. It resulted in a similar RMSE of 3.84 from the entire prediction set and
 495 3.77 and 3.91 within each block. This phenomenon emphasizes again that RMSE is affected solely by the magnitude
 496 of the error, which neglects the ability of the model to capture relative trends in intra-block or inter-block predictions.
 497 On the other hand, when the goal is to rank observations of interest rather than predict the absolute magnitude of the
 498 error, linearity-based metrics can provide more insights. The correlation r is an example showing its consistency across

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

524 3.5 Study 5: Label-Invariant Metrics Provide Balanced Assessment in Binary Classification

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

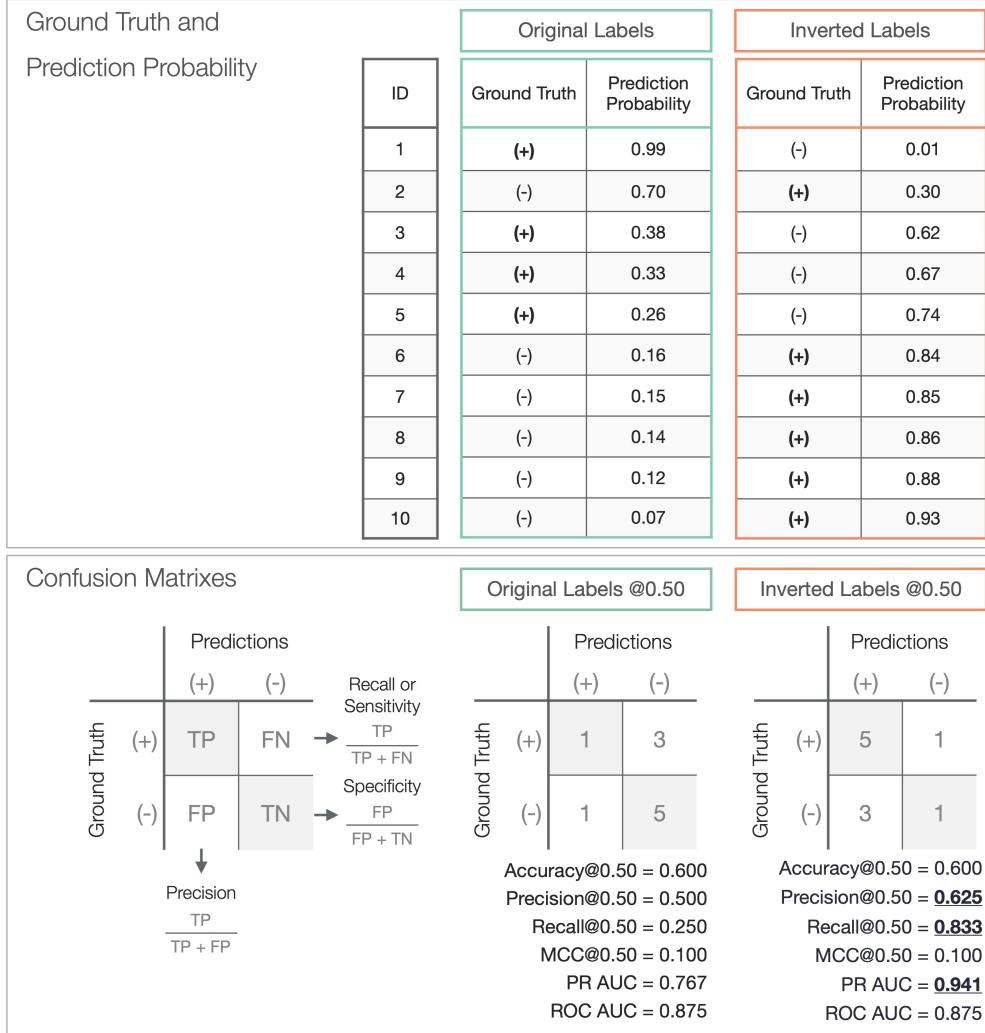


Figure 8: Simulated hypothetical example of binary classification. TP: true positive; FN: false negative; FP: false positive; TN: true negative; **Upper:** The ground truth and prediction probability. **Lower:** The confusion matrix of the prediction at a threshold of 0.5, followed by classification 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

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

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

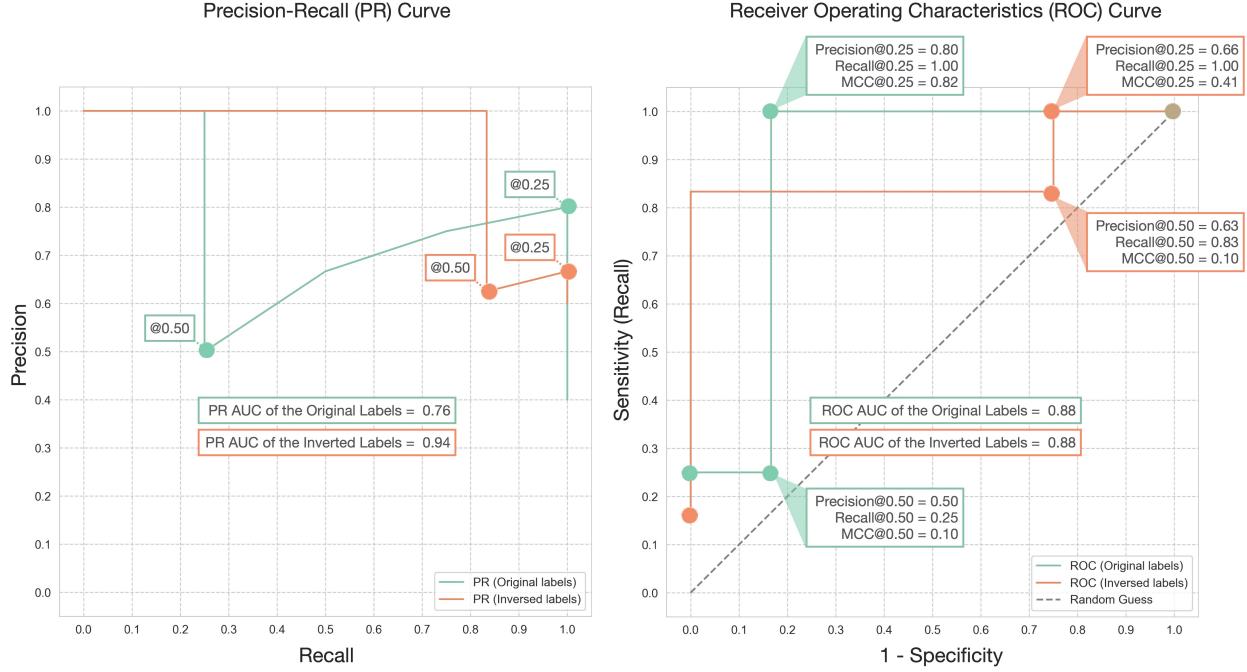


Figure 9: (**Left**) Precision-recall (PR) curve and (**Right**) Receiver operating characteristic (ROC) curve for the hypothetical example are displayed. The performance at confidence thresholds of 0.25 and 0.50 is highlighted. Original labels are marked in green, while inverted labels appear in orange.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

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

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

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

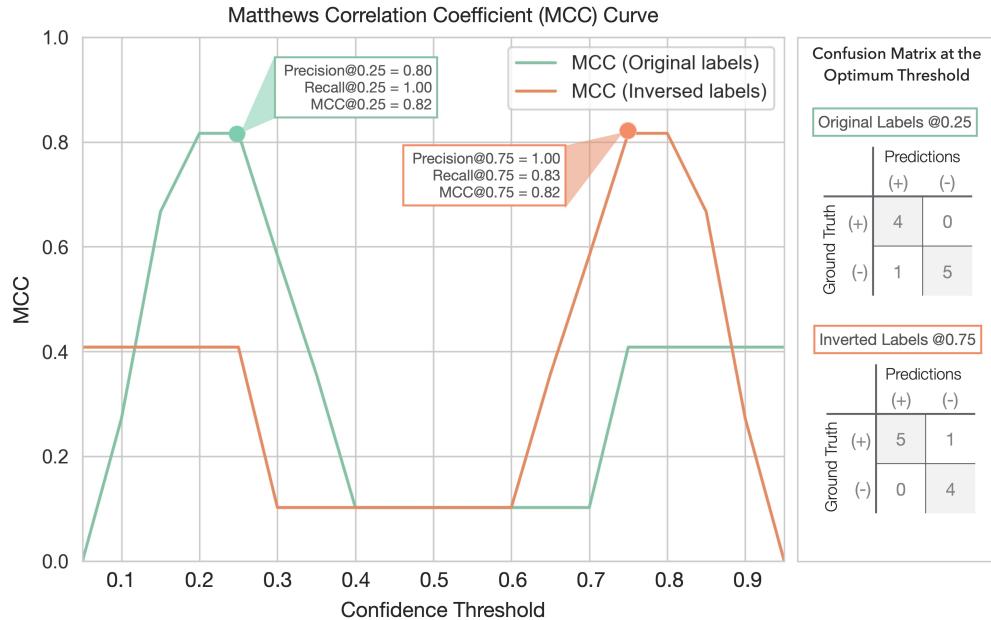


Figure 10: Matthews Correlation Coefficient (MCC) curve. A line chart plotting MCC at different thresholds for the hypothetical example. The optimal threshold is highlighted by the dot marks in green and orange for the original and inverted labels, respectively. The confusion matrix at the optimal threshold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

574 4 Conclusion

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

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701 **Appendix**

702 **Cross Validation**

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

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

707 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
 708 variable. The value of n corresponds to the total number of samples, while p represents the number of features. In
 709 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
 710 remaining folds make up the training set $\mathcal{D}_{\text{train}}$ (or \mathcal{D}_{-k}):

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

711 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 $f_{\mathcal{D}_{-k}}$.
 712 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
 713 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):

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

714 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
 715 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
 716 performance over all K folds. The model's generalization performance can be expressed as:

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

717 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
 718 all $\hat{g}(f_{\mathcal{D}_k})$ over K folds, which is also the definition of $\mathbb{E}[\hat{g}(f_{\mathcal{D}_k})]$.

719 Cross Validation Bias and Variance

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

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

723 For example, if RMSE is used as the performance metric, a positive validation bias suggests that the model validation
 724 procedure concludes a pessimistic estimation of the model performance, since the true performance is expected to be
 725 lower than the estimated performance. Another aspect of model validation is the variance of the estimated performance.
 726 For example, in a 5-fold cross-validation, there are five estimates of the model performance. The variance among these
 727 five estimates is known as validation variance. A high validation variance suggests that the performance is sensitive to
 728 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
 729 variance can be defined as:

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

730 Combining the Equations ?? and ??, the mean squared error (MSE) of the model validation can be decomposed as:

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

731 **Hyperparameter**

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

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

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

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

733 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
 734 denotes the sample size, and β is the coefficient vector. All three models aim to find the optimal β that minimizes their
 735 respective loss function, \mathcal{L} . In the regularized models (i.e., ridge and LASSO regression), the vector length of β is
 736 penalized in the loss function.

737 **Squared Correlation Coefficient r^2 and Determination Coefficient R^2**

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

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

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

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

745 where $SS_{\text{regression}}$ is the variation explained by the model and SS_{total} is the total sum of squares. Each Y_i and \hat{Y}_i are the
746 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
747 means. This proof highlights that under certain assumptions, r^2 and R^2 can indeed be equivalent, but such conditions
748 are specific to least squares regression where errors are normally distributed and predictions are unbiased estimates of
749 the actual values.