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Theory to Prediction: Hybrid Models for Binary Endogenous Variables in PLS-SEM Using Supervised Machine Learning

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Abstract
Theoretical explanation and out-of-sample prediction are both important in applied structural modeling. Partial least squares structural equation modeling (PLS-SEM) estimates relationships among latent-variable scores, but its ordinary least squares structural regressions are not directly suited to a binary endogenous outcome. We evaluate a hybrid workflow in which PLS-SEM latent scores are supplied to logistic regression (LR), linear and radial-kernel support vector machines (SVMs), and random forests (RFs). Eight open-source datasets were analyzed after the focal continuous endogenous score was dichotomized at the mean or median. Models were compared using 5-, 7-, and 10-fold cross-validation and 90:10, 80:20, and 70:30 train-test splits. Performance was assessed with sensitivity, specificity, accuracy, area under the receiver operating characteristic curve, Cohen's kappa, and the Matthews correlation coefficient. RF most frequently produced the highest cross-validation values, whereas held-out test performance varied across datasets and split ratios. Radial-kernel SVM was competitive in several datasets. The results show that supervised classifiers can extend a PLS-SEM workflow for constructed binary outcomes, but no classifier was uniformly superior. Model selection should therefore rely on prespecified tuning and rigorous out-of-sample validation.

Key Words: PLS-SEM; binary endogenous variable; supervised machine learning; hybrid model; predictive validation

1. Introduction

Prediction has become a central concern in applied research, but strong out-of-sample performance can be difficult to achieve in theory-driven models. Partial least squares structural equation modeling (PLS-SEM) is a multivariate method for estimating relationships among latent constructs and observed variables. It combines measurement and structural models and can represent mediation and moderation. PLS-SEM has been applied in international business (Shackman, 2013), the social sciences (Shanmugam & Marsh, 2015), management and hospitality research (Ali et al., 2018), accounting (Mondal et al., 2024), marketing (Sarstedt & Liu, 2024), information systems (Ramayah, 2024), and health research (Ansari et al., 2020; Sajid et al., 2020). Its use has expanded because it supports explanatory and prediction-oriented analyses and can accommodate complex models, non-normal data, and relatively small samples (Amusa & Hossana, 2024; Wong, 2011). Unlike covariance-based SEM, PLS-SEM emphasizes the explained variance (R^2) of endogenous constructs, which makes it attractive for prediction-oriented applications (Ali et al., 2018).

PLS-SEM commonly estimates each endogenous construct through a separate ordinary least squares regression. This approach is not directly suitable when an endogenous outcome is binary. Bodoff and Ho (2016) addressed such paths with logistic regression (LR). Although LR provides interpretable probability estimates, supervised machine-learning (ML) algorithms may capture nonlinear decision boundaries and interactions that a conventional main-effects LR model does not represent. Previous studies have combined ML with PLS-derived scores (Alzoubi, 2021; Yeganeh et al., 2012), but they have mainly examined continuous outcomes. This evidence motivates an evaluation of ML classifiers for binary endogenous outcomes within a PLS-SEM workflow.

This study develops and evaluates hybrid models that combine PLS-SEM latent scores with supervised ML classifiers. It compares linear and radial-basis-function support vector machines (SVMs) and random forests (RFs) with LR across eight secondary datasets, multiple train-test splits, and several cross-validation schemes. The study asks whether these classifiers improve predictive performance and whether their relative performance varies across datasets and validation designs.

2. Materials and Methods

Bodoff and Ho (2016) used LR to model a binary endogenous outcome from PLS-SEM scores. We extend this approach by evaluating supervised ML classifiers in the same setting. LR assumes that continuous predictors are linearly related to the log odds of the outcome unless nonlinear terms or interactions are specified. SVMs with nonlinear kernels and RFs can represent more flexible decision boundaries, although they introduce their own tuning and validation requirements. We therefore compare the methods empirically rather than assuming that one class of models will always perform better.

2.1. Implementation of the Conventional and Proposed Approaches

Figure 1 summarizes the conventional and proposed workflows. The conventional approach has two stages.

- First, the PLS-SEM measurement model is estimated and latent-variable scores are obtained.
- Second, the latent scores are used to estimate the structural paths. PLS-SEM estimates paths for continuous endogenous constructs, whereas LR estimates the paths leading to the binary endogenous outcome.
- The LR model is evaluated using sensitivity, specificity, accuracy, the area under the receiver operating characteristic curve (AUC), Cohen's kappa, and the Matthews correlation coefficient (MCC).

The proposed approach has three stages.

- First, as in the conventional workflow, the PLS-SEM measurement model is estimated to obtain latent-variable scores.
- Second, the binary outcome and the scores of its exogenous latent variables are supplied to a linear SVM, a radial-kernel SVM, and an RF classifier.
- Third, the hybrid models are evaluated with the same performance metrics as LR. Their results are compared across cross-validation schemes and train-test splits.

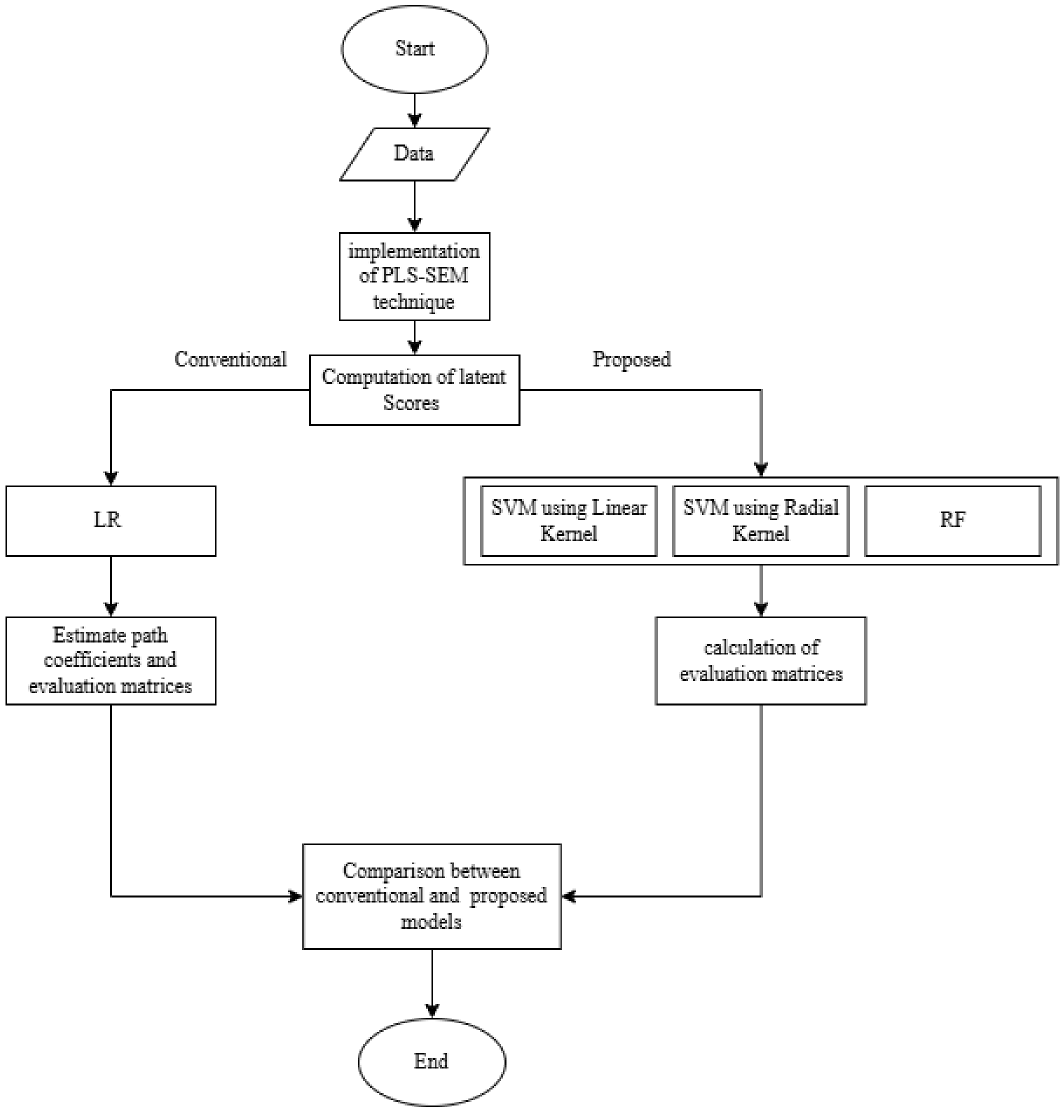

Figure 1. Conventional and proposed hybrid-model workflows

2.2. Data Sources and Software

We analyzed secondary datasets from several fields. Table 1 reports their sources and basic characteristics. All analyses were conducted in R version 4.5.0 using the seminr, caTools, caret, e1071, randomForest, mccr, Metrics, and pROC packages.

2.3. Dataset Preparation and Illustrative PLS-SEM Model

The eight selected datasets did not contain an originally binary endogenous construct. Following the general procedure used by Bodoff and Ho (2016), we dichotomized the score of the focal endogenous construct. We assessed the score distribution with the Shapiro-Wilk test. Scores with $p < 0.05$ were dichotomized at the median; otherwise, they were dichotomized at the mean. Median and mean splits discard information and can affect effect estimates and predictive performance (Rucker et al., 2015); therefore, the resulting outcomes should be interpreted as constructed binary endpoints rather than naturally binary variables.

Table 1. Summary of Datasets

Datasets	Field	References	Sample Size	Distribution of latent score	The decision for the dependent variable split
Dataset-1	Management and Marketing	Henseler et al. (2012)	30	Non-normal	Median
Dataset-2	Information System	Bodoff and Ho (2016)	250	Non-normal	Median
Dataset-3	Information Technology	(Hair Jr et al., 2021)	344	Non-normal	Median
Dataset-4	Tourism	Oliveira et al. (2020)	381	Non-normal	Median
Dataset-5	Marketing	Wong (2013)	400	Non-normal	Median
Dataset-6	Information Technology	Al-Gahtani et al. (2007)	722	Non-normal	Median
Dataset-7	Management Science	Garson (2016)	932	Normal	Mean
Dataset-8	Computing	(Anderson et al., 2011)	1190	Non-normal	Median

Figure 2 illustrates a PLS-SEM model from Dataset 8. The published measurement and structural specifications were retained, except that the focal endogenous construct (ASU) was dichotomized at the median as described above.

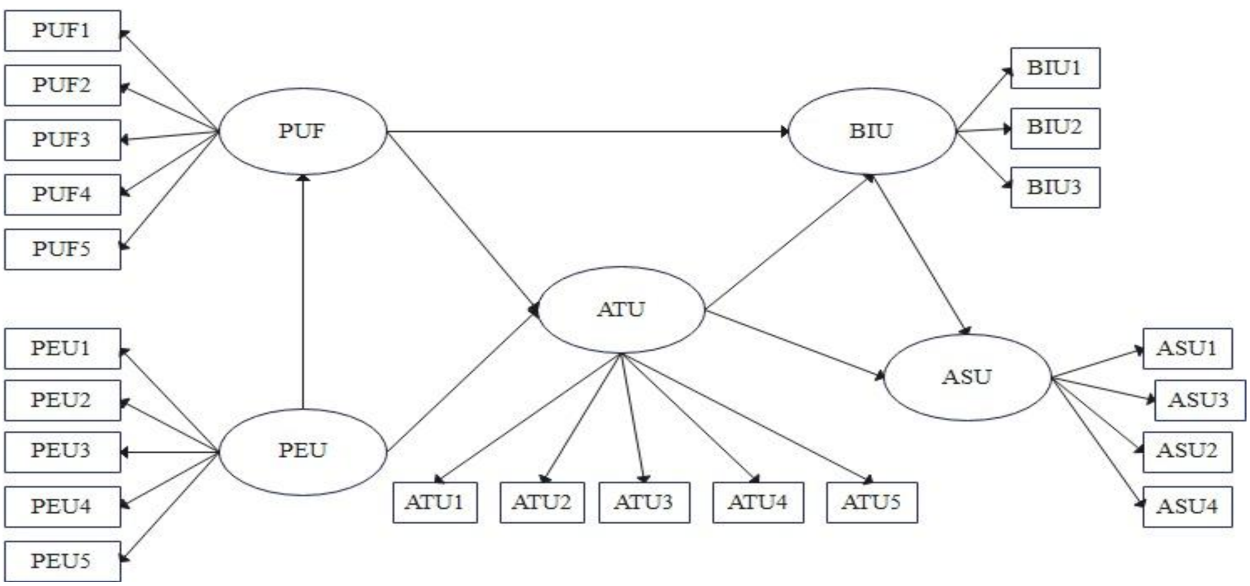

Figure 2. PLS-SEM model for Dataset 8

2.4. Statistical Model and Machine-Learning Algorithms

LR served as the baseline classifier. The alternative models were linear SVM, radial-kernel SVM, and RF. We use the term radial-kernel SVM consistently throughout the manuscript. Artificial neural networks were not evaluated because several datasets were small, making reliable training and tuning difficult.

LR is a statistical model that uses the sigmoid function to provide probabilities for a binary outcome variable. This sigmoid function is $P = 1/(1 + \exp(-y))$. is generally not used for measuring complex relationships like non-linear relationships of $(log\, p/(1 - p))$ with quantitative independent variable Menard (2010). While SVM is one of the algorithms that has strong mathematical foundations and can deal with linear as well as non-linear relationships in the model. It is employed primarily for classification tasks, though it can also handle regression problems. The algorithm functions by constructing a boundary, or hyperplane, in various orientations to separate data points belonging to different classes. The dimensionality of this hyperplane is determined by the number of input features. For instance, with two input features, the hyperplane is simply a line, while with three, it becomes a plane. The core objective of the SVM algorithm is to identify the optimal hyperplane that maximises the margin between different data classes in an N-dimensional space Guido et al. (2024). Further, it can work in higher-dimensional space using kernel functions. In this study, linear and non-linear kernels are used. The linear kernel uses the following equation.

$$k\left(x, x^{/}\right) = f(x^{/}).f(x) \tag{1}$$

Where x, and $x^{/}$ are n-dimensional inputs, and k represents the kernel function. The non-linear (radial) kernel uses the following equation.

$$k\left(x, x^{/}\right) = \exp\ \left((-1/2\delta^2) \times \left\|x - x^{/}\right\|^2\right), \delta > 0 \tag{2}$$

Here δ is a free parameter and $x - x^{/}$ is the Euclidean distance between two feature vectors.

RF is an ensemble classifier that combines bootstrap sampling with random feature selection. Each tree is fitted to a bootstrap sample, and a random subset of predictors is considered at each split. Classification is based on the majority vote across trees. Aggregating decorrelated trees generally reduces prediction variance relative to a single decision tree (Kulkarni & Sinha, 2012; Liu et al., 2012; Zhang & Ma, 2012). RF can represent nonlinearities and interactions, but its performance still depends on tuning, sample size, class balance, and validation design (Helmud et al., 2024).

2.5. Model Validation and Performance Metrics

We evaluated the models using three train-test splits (90:10, 80:20, and 70:30) and 5-, 7-, and 10-fold cross-validation. Sensitivity is the proportion of positive cases correctly classified, whereas specificity is the proportion of negative cases correctly classified (Vanacore et al., 2024; Wong & Lim, 2011). Accuracy is the proportion of all observations classified correctly; it is not generally equal to the unweighted mean of sensitivity and specificity. AUC summarizes discrimination across classification thresholds and is not the product of sensitivity and specificity. Cohen's kappa measures agreement between observed and predicted classes beyond chance. MCC summarizes the association between observed and predicted binary classes and ranges from -1 to 1. Higher sensitivity, specificity, accuracy, AUC, kappa, and MCC indicate better performance, although their interpretation depends on class prevalence and the decision threshold.

3. Results

This section reports results for eight datasets (Table 1). Tables 2-9 present LR and ML performance under cross-validation and the three train-test splits. Values exceeding the LR baseline are shown in bold, and the highest value for each metric is shown in blue. Because no inferential comparisons or uncertainty intervals were reported, differences are described as numerical rather than statistically significant.

Dataset 1 had only 30 observations. Seven- and ten-fold cross-validation and the 70:30 split were not reported because some resamples produced computational failures. The LR baseline yielded sensitivity, specificity, accuracy, and AUC values of approximately 0.93. Linear and radial-kernel SVMs produced results similar to LR under the reported validation settings. RF produced the highest cross-validation accuracy and AUC (approximately 0.96) and also exceeded the other models for the reported train-test splits. These estimates are unstable because each test set contains very few observations.

Table 2. Cross-Validation, Training and Testing Results of the Dataset-1

		AUC	**MCC**	**Accuracy**	**Kappa**	**Sensitivity**	**Specificity**
LR	**Baseline**	0.9333	0.8667	0.9333	0.8667	0.9333	0.9333
		Cross-Validation					
SVM with Linear Kernel	**10-fold**	0.9333	0.8667	0.9333	0.8667	0.9333	0.9333
	7-fold	0.9333	0.8667	0.9333	0.8667	0.9333	0.9333
	5-fold	0.9333	0.8667	0.9333	0.8667	0.9333	0.9333
SVM using Radial kernel	**10-fold**	0.9000	0.8018	0.9000	0.8000	0.8667	0.9333
	7-fold	0.9000	0.8018	0.9000	0.8000	0.8667	0.9333

	5-fold	0.9000	0.8018	0.9000	0.8000	0.8667	0.9333
RF	**10-fold**	**0.9667**	**0.9354**	**0.9667**	**0.9333**	**1.0000**	0.9333
	7-fold	0.9333	0.8667	0.9333	0.8667	0.9333	0.9333
	5-fold	0.9333	0.8667	0.9333	0.8667	0.9333	0.9333
Training Results							
SVM using Linear Kernel	**90:10**	0.8929	0.7877	0.8929	0.7857	0.8571	0.9286
	80:20	0.9167	0.8333	0.9167	0.8333	0.9167	0.9167
SVM using Radial kernel	**90:10**	0.8929	0.7877	0.8929	0.7857	0.8571	0.9286
	80:20	0.8750	0.7526	0.875	0.7500	0.8333	0.9167
RF	**90:10**	**1.0000**	**1.0000**	**1.0000**	**1.0000**	**1.0000**	**1.0000**
	80:20	**1.0000**	**1.0000**	**1.0000**	**1.0000**	**1.0000**	**1.0000**
Testing Results							
SVM using Linear Kernel	**90:10**	**1.0000**	**1.0000**	**1.0000**	**1.0000**	**1.0000**	**1.0000**
	80:20	**1.0000**	**1.0000**	**1.0000**	**1.0000**	**1.0000**	**1.0000**
SVM using Radial kernel	**90:10**	**1.0000**	**1.0000**	**1.0000**	**1.0000**	**1.0000**	**1.0000**
	80:20	**1.0000**	**1.0000**	**1.0000**	**1.0000**	**1.0000**	**1.0000**
RF	**90:10**	**1.0000**	**1.0000**	**1.0000**	**1.0000**	**1.0000**	**1.0000**
	80:20	**1.0000**	**1.0000**	**1.0000**	**1.0000**	**1.0000**	**1.0000**

For Dataset 2, RF produced the highest cross-validation values at each reported fold count. Results varied across the 90:10 and 80:20 train-test splits, whereas both SVM variants exceeded LR on some metrics. Dataset 3 showed a similar pattern: RF generally produced the highest values, but performance depended on the validation design and split.

Table 3. Cross-Validation, Training and Testing Results of the Dataset-2

		AUC	MCC	Accuracy	Kappa	Sensitivity	Specificity
LR	**Baseline**	0.7256	0.4473	0.7280	0.4463	0.7826	0.6607
Cross-Validation							
SVM using Linear Kernel	**10-fold**	0.7253	**0.4552**	**0.7320**	**0.4540**	**0.7899**	0.6607
	7-fold	0.7253	**0.4552**	**0.7320**	**0.4540**	**0.7899**	0.6607
	5-fold	0.7253	**0.4552**	**0.7320**	**0.4540**	**0.7899**	0.6607
SVM using Radial Kernel	**10-fold**	0.7155	0.4383	0.7240	0.4358	**0.7971**	0.6339
	7-fold	0.7152	**0.4604**	**0.7320**	0.4427	**0.8768**	0.5536
	5-fold	0.7152	**0.4604**	**0.7320**	0.4427	**0.8768**	0.5536
RF	**10-fold**	**0.8257**	**0.6519**	**0.8280**	**0.6519**	**0.8478**	**0.8036**
	7-fold	**0.8229**	**0.6433**	**0.8240**	**0.6429**	**0.8551**	**0.7857**
	5-fold	**0.8346**	**0.6687**	**0.8360**	**0.6687**	**0.8478**	**0.8214**
Training Results							
SVM using Linear Kernel	**90:10**	**0.7290**	**0.4669**	**0.7378**	**0.4636**	**0.8145**	0.6436
	80:20	0.7167	0.4409	0.7250	0.4382	**0.8000**	0.6333
	70:30	0.7110	0.4292	0.7200	0.4268	**0.7938**	0.6282
SVM using Radial Kernel	**90:10**	0.6957	0.4143	0.7111	0.4013	**0.8468**	0.5446
	80:20	0.6793	0.3809	0.6950	0.3679	**0.8364**	0.5222
	70:30	0.7177	**0.4735**	**0.7371**	**0.4501**	**0.8969**	0.5385
RF	**90:10**	**0.8383**	**0.6766**	**0.8400**	**0.6766**	**0.8548**	**0.8218**
	80:20	**0.7919**	**0.5955**	**0.8000**	**0.5910**	**0.8727**	**0.7111**
	70:30	**0.7331**	**0.5162**	**0.7543**	**0.4839**	**0.9278**	0.5385
Testing Results							
SVM using Linear Kernel	**90:10**	0.6591	0.3290	0.6400	0.3034	0.5000	**0.8182**
	80:20	**0.7435**	**0.4835**	**0.7400**	**0.4800**	0.7143	**0.7727**
	70:30	**0.7457**	**0.4903**	**0.7467**	**0.4902**	0.7561	**0.7353**

SVM using Radial Kernel	**90:10**	**0.7305**	**0.4610**	0.7200	**0.4479**	**0.6429**	**0.8182**
	80:20	**0.7792**	**0.5562**	**0.7800**	**0.5557**	**0.7857**	**0.7727**
	70:30	0.7184	**0.4662**	**0.7330**	**0.4481**	**0.8780**	0.5588
RF	**90:10**	**0.8214**	**0.6648**	**0.8000**	**0.613**	**0.6429**	**1.0000**
	80:20	0.7208	0.4387	0.7200	0.4373	0.7143	**0.7273**
	70:30	0.7037	0.4399	0.7200	0.4190	**0.8780**	0.5294

Table 4. Cross-Validation, Training and Testing Results of the Dataset-3

		AUC	MCC	Accuracy	Kappa	Sensitivity	Specificity
LR	**Baseline**	0.7774	0.5535	0.7791	0.5533	0.8085	0.7436
			Cross-Validation				
SVM using Linear Kernel	**10-fold**	0.7691	0.5411	0.7733	0.5405	**0.8138**	0.7244
	7-fold	0.7691	0.5411	0.7733	0.5405	**0.8138**	0.7244
	5-fold	0.7691	0.5411	0.7733	0.5405	**0.8138**	0.7244
SVM using Radial Kernel	**10-fold**	0.7648	0.5349	0.7703	0.5334	**0.8245**	0.7051
	7-fold	0.7648	0.5349	0.7703	0.5334	**0.8245**	0.7051
	5-fold	0.7685	0.5409	0.7733	0.5400	**0.8191**	0.7179
RF	**10-fold**	**0.8965**	**0.7945**	**0.8983**	**0.7944**	**0.9149**	**0.8782**
	7-fold	**0.8933**	**0.7886**	**0.8953**	**0.7884**	**0.9149**	**0.8718**
	5-fold	**0.8720**	**0.7475**	**0.8750**	**0.7469**	**0.9043**	**0.8397**
			Training Results				
SVM using Linear Kernel	**90:10**	0.7175	0.4339	0.7184	0.4336	0.7278	0.7071
	80:20	0.7393	0.4844	0.7455	0.4825	0.8067	0.6720
	70:30	0.7410	0.4868	0.7469	0.4854	0.8030	0.6789
SVM using Radial Kernel	**90:10**	0.7345	0.4751	0.7411	0.4731	0.8047	0.6643
	80:20	0.7647	0.5364	0.7709	0.5340	**0.8333**	0.6960
	70:30	**0.8139**	**0.6407**	**0.8216**	**0.6355**	**0.8939**	0.7339
RF	**90:10**	**0.9483**	**0.9031**	**0.9515**	**0.9015**	**0.9822**	**0.9143**
	80:20	**0.8540**	**0.7138**	**0.8582**	**0.7123**	**0.9000**	**0.8080**
	70:30	**0.8110**	**0.6312**	**0.8174**	**0.6279**	**0.8788**	0.7431
			Testing Results				
SVM using Linear Kernel	**90:10**	**0.8898**	**0.7771**	**0.8857**	**0.7720**	**0.8421**	**0.9375**
	80:20	**0.8565**	**0.7101**	**0.8551**	**0.7089**	**0.8421**	**0.8710**
	70:30	**0.8026**	**0.6078**	**0.8058**	**0.6073**	**0.8393**	**0.7660**
SVM using Radial Kernel	**90:10**	**0.8849**	**0.7697**	**0.8857**	**0.7697**	**0.8947**	**0.8750**
	80:20	**0.8565**	**0.7101**	**0.8551**	**0.7089**	**0.8421**	**0.8710**
	70:30	0.6605	0.3297	0.6699	0.3255	0.7679	0.5532
RF	**90:10**	**0.9112**	**0.8278**	**0.9143**	**0.8264**	**0.9474**	**0.8750**
	80:20	**0.8141**	**0.6250**	**0.8116**	**0.6226**	0.7895	**0.8387**
	70:30	0.7690	0.5498	0.7767	0.5445	**0.8571**	0.6809

For Dataset 4, the RF-based PLS-SEM workflow produced higher accuracy, AUC, kappa, MCC, sensitivity, and specificity than the LR baseline in cross-validation. At 10-fold cross-validation, RF yielded an AUC of 0.98. Performance varied across train-test splits. Dataset 5 showed a similar pattern, with RF generally exceeding the LR and SVM models.

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Table 5. Cross-Validation, Training and Testing Results of the Dataset-4

		AUC	MCC	Accuracy	Kappa	Sensitivity	Specificity
LR	**Baseline**	0.8324	0.6643	0.8320	0.6640	0.8482	0.8158
		Cross-Validation					
SVM using Linear Kernel	**10-fold**	0.8294	0.6588	0.8294	0.6588	0.8325	**0.8263**
	7-fold	0.8294	0.6588	0.8294	0.6588	0.8325	**0.8263**
	5-fold	0.8294	0.6588	0.8294	0.6588	0.8325	**0.8263**
SVM using Radial Kernel	**10-fold**	0.8215	0.6432	0.8215	0.6430	0.8325	0.8105
	7-fold	**0.8452**	**0.6903**	**0.8451**	**0.6903**	0.8429	**0.8474**
	5-fold	**0.8583**	**0.7172**	**0.8583**	**0.7166**	0.8377	**0.8789**
RF	**10-fold**	**0.9816**	**0.9633**	**0.9816**	**0.9633**	**0.9843**	**0.9789**
	7-fold	**0.9370**	**0.8741**	**0.9370**	**0.8740**	**0.9319**	**0.9421**
	5-fold	**0.9186**	**0.8376**	**0.9186**	**0.8373**	**0.9058**	**0.9316**
		Training Results					
SVM using Linear Kernel	**90:10**	0.8251	0.6502	0.8251	0.6502	0.8198	**0.8304**
	80:20	0.8262	0.6525	0.8262	0.6524	0.8301	**0.8224**
	70:30	0.8240	0.6481	0.8240	0.6480	0.8134	**0.8346**
SVM Using Radial Kernel	**90:10**	**0.8397**	**0.6796**	**0.8397**	**0.6793**	0.8256	**0.8538**
	80:20	**0.8459**	**0.6919**	**0.8459**	**0.6918**	0.8366	**0.8553**
	70:30	0.8277	0.6555	0.8277	0.6554	0.8358	**0.8195**
RF	**90:10**	**0.9300**	**0.8601**	**0.9300**	**0.8601**	**0.9302**	**0.9298**
	80:20	**0.8853**	**0.7707**	**0.8852**	**0.7705**	**0.8758**	**0.8947**
	70:30	**0.8839**	**0.7678**	**0.8839**	**0.7678**	**0.8881**	**0.8797**
		Testing Results					
SVM using Linear Kernel	**90:10**	**0.8684**	**0.7462**	**0.8684**	**0.7368**	**0.9474**	0.7895
	80:20	**0.8421**	**0.6842**	**0.8421**	**0.6842**	**0.8421**	**0.8421**
	70:30	**0.8333**	**0.6668**	**0.8333**	**0.6667**	0.8421	**0.8246**
SVM using Radial Kernel	**90:10**	**0.9211**	**0.8528**	**0.9211**	**0.8421**	**1.0000**	**0.8421**
	80:20	**0.8816**	**0.7655**	**0.8816**	**0.7632**	**0.8421**	**0.9211**
	70:30	**0.8596**	**0.7193**	**0.8596**	**0.7193**	**0.8596**	**0.8596**
RF	**90:10**	**0.9211**	**0.8528**	**0.9211**	**0.8421**	**1.0000**	**0.8421**
	80:20	**0.8553**	**0.7108**	**0.8553**	**0.7105**	**0.8421**	**0.8684**
	70:30	**0.8421**	**0.6846**	**0.8421**	**0.6842**	**0.8596**	**0.8246**

Table 6. Cross-Validation, Training and Testing Results of the Dataset-5

		AUC	MCC	Accuracy	Kappa	Sensitivity	Specificity
LR	**Baseline**	0.7725	0.5450	0.7725	0.5450	0.7750	0.7700
		Cross-Validation					
SVM using Linear Kernel	**10-fold**	0.7675	0.5352	0.7675	0.5350	**0.7800**	0.7550
	7-fold	0.7675	0.5352	0.7675	0.5350	**0.7800**	0.7550
	5-fold	0.7675	0.5352	0.7675	0.5350	**0.7800**	0.7550
SVM using Radial Kernel	**10-fold**	**0.8625**	**0.7252**	**0.8625**	**0.7250**	**0.8500**	**0.8750**
	7-fold	**0.8675**	**0.7351**	**0.8675**	**0.7350**	**0.8600**	**0.8750**
	5-fold	**0.8525**	**0.7054**	**0.8525**	**0.7050**	**0.8350**	**0.8700**
RF	**10-fold**	**0.9700**	**0.9400**	**0.9700**	**0.9400**	**0.9650**	**0.9750**
	7-fold	**0.9800**	**0.9600**	**0.9800**	**0.9600**	**0.9850**	**0.9750**
	5-fold	**0.9400**	**0.8807**	**0.9400**	**0.8800**	**0.9200**	**0.9600**
		Training Results					
SVM using Linear Kernel	**90:10**	**0.7778**	**0.5568**	**0.7778**	**0.5556**	0.7444	**0.8111**
	80:20	**0.7750**	**0.5516**	**0.7750**	**0.5500**	0.7375	**0.8125**
	70:30	**0.7750**	**0.5507**	**0.7750**	**0.5500**	0.7500	**0.8000**
SVM using	**90:10**	**0.8361**	**0.6722**	**0.8361**	**0.6722**	**0.8333**	**0.8389**

Radial Kernel	**80:20**	**0.7875**	**0.5754**	**0.7875**	**0.5750**	**0.8063**	0.7688
	70:30	**0.8071**	**0.6207**	**0.8071**	**0.6143**	**0.8786**	0.7357
RF	**90:10**	**0.8611**	**0.7233**	**0.8611**	**0.7222**	**0.8333**	**0.8889**
	80:20	**0.8719**	**0.7449**	**0.8719**	**0.7437**	**0.8438**	**0.9000**
	70:30	**0.8107**	**0.6216**	**0.8107**	**0.6214**	**0.8214**	**0.8000**
Testing Results							
SVM using Linear Kernel	**90:10**	**0.7750**	**0.5507**	**0.7750**	**0.5500**	**0.8000**	0.7500
	80:20	0.7625	0.5265	0.7625	0.5250	**0.8000**	0.7250
	70:30	**0.7750**	**0.5563**	**0.7750**	**0.5500**	**0.8500**	0.7000
SVM using Radial Kernel	**90:10**	**0.8250**	**0.6574**	**0.8250**	**0.6500**	**0.9000**	0.7500
	80:20	0.7500	0.5103	0.7500	0.5000	**0.8500**	0.6500
	70:30	0.7250	0.4744	0.7250	0.4500	**0.8833**	0.5667
RF	**90:10**	**0.8500**	**0.7036**	**0.8500**	**0.7000**	**0.9000**	**0.8000**
	80:20	**0.8250**	**0.6533**	**0.8250**	**0.6500**	**0.8750**	0.7000
	70:30	0.7583	0.5256	0.7583	0.5167	**0.8500**	0.6667

Table 7. Cross-Validation, Training and Testing Results of the Dataset-6

		AUC	MCC	Accuracy	Kappa	Sensitivity	Specificity
LR	**Baseline**	0.6629	0.3254	0.6620	0.3247	0.6349	0.6901
Cross-Validation							
SVM using Linear Kernel	**10-fold**	**0.6640**	**0.3284**	**0.6634**	**0.3275**	0.6322	**0.6958**
	7-fold	0.6611	0.3227	0.6607	0.3219	0.6322	0.6901
	5-fold	**0.6668**	**0.3342**	**0.6662**	**0.3331**	0.6322	**0.7014**
SVM using Radial Kernel	**10-fold**	**0.6787**	**0.3621**	**0.6801**	**0.3584**	**0.7548**	0.6028
	7-fold	**0.6787**	**0.3621**	**0.6801**	**0.3584**	**0.7548**	0.6028
	5-fold	**0.6851**	**0.3810**	**0.6870**	**0.3715**	**0.8011**	0.5690
RF	**10-fold**	**0.8491**	**0.6980**	**0.8490**	**0.6980**	**0.8474**	**0.8507**
	7-fold	**0.8408**	**0.6815**	**0.8407**	**0.6814**	**0.8365**	**0.8451**
	5-fold	**0.8490**	**0.6979**	**0.8490**	**0.6908**	**0.8529**	**0.8451**
Training Results							
SVM using Linear Kernel	**90:10**	0.6589	0.3182	0.6585	0.3175	0.6303	0.6875
	80:20	0.6614	0.3232	0.6609	0.3224	0.6327	0.6901
	70:30	0.6559	0.3121	0.6554	0.3114	0.6304	0.6815
SVM using Radial Kernel	**90:10**	**0.6784**	**0.3655**	**0.6800**	**0.3578**	**0.7848**	0.5719
	80:20	**0.6793**	**0.3728**	**0.6817**	**0.3603**	**0.8129**	0.5458
	70:30	0.6530	0.3065	0.6535	0.3063	**0.6770**	0.6290
RF	**90:10**	**0.7998**	**0.5999**	**0.8000**	**0.5998**	**0.8152**	**0.7844**
	80:20	**0.7416**	**0.4847**	**0.7422**	**0.4837**	**0.7789**	**0.7042**
	70:30	**0.7457**	**0.4940**	**0.7465**	**0.4921**	**0.7938**	**0.6976**
Testing Results							
SVM using Linear Kernel	**90:10**	**0.7251**	**0.4588**	**0.7222**	**0.4474**	0.6216	**0.8286**
	80:20	**0.6889**	**0.3851**	**0.6875**	**0.3767**	0.5890	**0.7887**
	70:30	**0.6828**	**0.3676**	**0.6820**	**0.3650**	0.6273	**0.7383**
SVM using Radial Kernel	**90:10**	**0.7490**	**0.4996**	**0.7500**	**0.4988**	**0.7838**	**0.7143**
	80:20	**0.7220**	**0.4443**	**0.7222**	**0.4441**	**0.7397**	**0.7042**
	70:30	**0.7055**	**0.4117**	**0.7051**	**0.4106**	**0.6727**	**0.7383**
RF	**90:10**	**0.7514**	**0.5043**	**0.7500**	**0.5012**	**0.7027**	**0.8000**
	80:20	0.6603	0.3218	0.6597	0.3202	0.6164	**0.7042**
	70:30	**0.6959**	**0.3918**	**0.6959**	**0.3917**	**0.6909**	**0.7009**

The ML-based workflows also produced higher values than LR for several metrics in Datasets 6-8 (Tables 7-9). In Datasets 7 and 8, the radial-kernel SVM exceeded the linear SVM on several measures, which is consistent with—but *does not establish—the presence of nonlinear decision boundaries. Across the eight datasets, RF most consistently achieved the highest cross-validation values.*

Table 8. Cross-Validation, Training and Testing Results of the Dataset-7

		AUC	MCC	Accuracy	Kappa	Sensitivity	Specificity
LR	**Baseline**	0.7274	0.4548	0.7275	0.4548	0.7217	0.7331
			Cross-Validation				
SVM using Linear Kernel	**10-fold**	**0.7294**	**0.4591**	**0.7296**	**0.4590**	0.7196	**0.7394**
	7-fold	**0.7305**	**0.4612**	**0.7307**	**0.4612**	0.7196	**0.7415**
	5-fold	**0.7305**	**0.4612**	**0.7307**	**0.4612**	0.7196	**0.7415**
SVM using Radial Kernel	**10-fold**	**0.7282**	**0.4571**	**0.7285**	**0.4567**	0.7022	**0.7542**
	7-fold	**0.7323**	**0.4664**	**0.7328**	**0.4651**	0.6913	**0.7733**
	5-fold	**0.7322**	**0.4671**	**0.7328**	**0.4649**	0.6804	**0.7839**
RF	**10-fold**	**0.9001**	**0.8004**	**0.9002**	**0.8004**	**0.8935**	**0.9068**
	7-fold	**0.8882**	**0.7771**	**0.8884**	**0.7767**	**0.8717**	**0.9047**
	5-fold	**0.9131**	**0.8261**	**0.9131**	**0.8261**	**0.9109**	**0.9153**
			Training Results				
SVM using Linear Kernel	**90:10**	**0.7283**	**0.4566**	**0.7282**	**0.4565**	**0.7319**	0.7247
	80:20	0.7238	0.4477	0.7239	0.4477	**0.7228**	0.7249
	70:30	**0.7315**	**0.4631**	**0.7316**	**0.4631**	**0.7267**	**0.7364**
SVM using Radial Kernel	**90:10**	**0.7480**	**0.4977**	**0.7485**	**0.4965**	0.7101	**0.7859**
	80:20	0.7263	0.4529	0.7265	0.4528	0.7092	**0.7434**
	70:30	0.7264	**0.4555**	0.7270	0.4532	0.6739	**0.7788**
RF	**90:10**	**0.7781**	**0.5566**	**0.7783**	**0.5564**	**0.7609**	**0.7953**
	80:20	**0.7573**	**0.5146**	**0.7574**	**0.5146**	**0.7500**	**0.7646**
	70:30	**0.7698**	**0.5398**	**0.7699**	**0.5397**	**0.7547**	**0.7848**
			Testing Results				
SVM using Linear Kernel	**90:10**	**0.7632**	**0.5271**	**0.7634**	**0.5266**	**0.7391**	**0.7872**
	80:20	**0.7523**	**0.5060**	**0.7527**	**0.5050**	0.7174	**0.7872**
	70:30	**0.7386**	**0.4799**	**0.7393**	**0.4778**	0.6884	**0.7887**
SVM using Radial Kernel	**90:10**	**0.7414**	**0.4851**	**0.7419**	**0.4833**	0.6957	**0.7872**
	80:20	**0.7523**	**0.5060**	**0.7527**	**0.5050**	**0.7174**	**0.7872**
	70:30	**0.7309**	**0.4693**	**0.7321**	**0.4629**	**0.6449**	**0.8169**
RF	**90:10**	**0.7417**	**0.4840**	**0.7419**	**0.4836**	0.7174	**0.7660**
	80:20	**0.7471**	**0.4946**	**0.7473**	**0.4944**	**0.7283**	**0.7660**
	70:30	**0.7386**	**0.4799**	**0.7393**	**0.4778**	0.6884	**0.7887**

Table 9. Cross-Validation, Training and Testing Results of the Dataset-8

		AUC	MCC	Accuracy	Kappa	Sensitivity	Specificity
LR	**Baseline**	0.6239	0.2459	0.6218	0.2440	0.5611	0.6830
			Cross-Validation				
SVM using Linear Kernel	**10-fold**	0.6079	0.2223	0.6076	0.2158	0.4891	**0.7268**
	7-fold	0.6080	0.2223	0.6076	0.2158	0.4891	**0.7268**
	5-fold	0.6087	0.2211	0.6084	0.2173	0.5176	**0.6998**
SVM using Radial Kernel	**10-fold**	**0.6434**	**0.2922**	**0.6437**	**0.2869**	**0.7387**	0.5481
	7-fold	**0.6460**	**0.2949**	**0.6462**	**0.2921**	**0.7152**	0.5767
	5-fold	**0.6468**	**0.2966**	**0.6471**	**0.2938**	**0.7169**	0.5767
RF	**10-fold**	**0.7917**	**0.5873**	**0.7916**	**0.5833**	**0.7621**	**0.8212**
	7-fold	**0.7849**	**0.5697**	**0.7849**	**0.5697**	**0.7856**	**0.7841**
	5-fold	**0.7807**	**0.5617**	**0.7807**	**0.5614**	**0.7655**	**0.7960**
			Training Results				
	90:10	0.6053	0.2152	0.6050	0.2105	0.5028	**0.7079**

SVM using Linear Kernel	**80:20**	0.6127	0.2287	0.6124	0.2253	0.5293	**0.6962**
	70:30	0.6163	0.2416	0.6158	0.2324	0.4809	**0.7518**
SVM using Radial Kernel	**90:10**	**0.6422**	**0.2868**	**0.6424**	**0.2845**	**0.7058**	0.5787
	80:20	**0.6455**	**0.2996**	**0.6460**	**0.2913**	**0.7636**	0.5274
	70:30	**0.6443**	**0.2933**	**0.6447**	**0.2889**	**0.7321**	0.5566
RF	**90:10**	**0.6731**	**0.3471**	**0.6732**	**0.3463**	**0.7076**	0.6386
	80:20	**0.6689**	**0.3389**	**0.6691**	**0.3380**	**0.7071**	0.6308
	70:30	**0.6559**	**0.3133**	**0.6555**	**0.3106**	**0.7225**	0.5880
Testing Results							
SVM using Linear Kernel	**90:10**	0.6059	0.2167	0.6050	0.2115	0.5000	**0.7119**
	80:20	0.5924	0.1906	0.5924	0.1849	0.4706	**0.7143**
	70:30	0.5859	0.1799	0.5854	0.1716	0.4358	**0.7360**
SVM using Radial Kernel	**90:10**	**0.6463**	**0.2973**	**0.6471**	**0.2931**	**0.7333**	0.5593
	80:20	**0.6261**	**0.2561**	**0.6261**	**0.2521**	**0.7143**	0.5378
	70:30	**0.6468**	**0.2975**	**0.6471**	**0.2938**	**0.7263**	0.5674
RF	**90:10**	**0.6298**	**0.2612**	**0.6303**	**0.2598**	**0.6833**	0.5763
	80:20	0.6218	0.2442	0.6218	0.2437	**0.6555**	0.5882
	70:30	**0.6356**	**0.2743**	**0.6359**	**0.2714**	**0.7095**	0.5618

Table 10. Overall Summary of the Results for all Datasets

	Training			**Testing**			**Cross-Validation**		
Techniques	**90:10**	**80:20**	**70:30**	**90:10**	**80:20**	**70:30**	**10-fold**	**7-fold**	**5-fold**
SVM using Linear Kernel	3	1	2	6	6	6	3	2	3
SVM using Radial Kernel	5	4	4	8	7	5	4	5	5
RF	8	8	7	8	5	4	8	7	7

Table 10 summarizes how often each classifier exceeded the LR baseline in Tables 2-9. RF did so most frequently in cross-validation and training samples, but its advantage was less consistent in held-out test samples. The radial-kernel SVM ranked second by this count. These frequencies summarize the observed datasets and should not be interpreted as formal evidence that one algorithm is universally superior.

4. Discussion

This study evaluated hybrid PLS-SEM classification workflows for a constructed binary endogenous outcome. Latent scores obtained from PLS-SEM were supplied to linear SVM, radial-kernel SVM, RF, and conventional LR classifiers. Across the eight datasets, RF most often produced the highest cross-validation metrics. Performance in held-out test samples was less consistent and varied with the train-test split.

Previous studies have reported that ML models can outperform conventional LR in some prediction tasks (Al-Imran et al., 2024; Sajid, Almehmadi, et al., 2021; Sajid et al., 2022). Such advantages are context-dependent and require appropriate tuning and validation. Sample size was therefore an important concern in the present study, because PLS-SEM is often applied to relatively small samples (Wicaksono et al., 2024), whereas flexible ML models can require substantially more data (Tsegaye et al., 2025). In Dataset 1 (n = 30), RF and SVM sometimes exceeded LR, but the very small validation samples make those differences imprecise. The results do not establish equivalence or superiority for very small samples.

We selected SVM and RF from the wider range of available supervised-learning methods because both can represent nonlinear classification boundaries and are commonly used with small-to-moderate datasets. Artificial neural networks were excluded because their training and tuning generally require more data (Dastres & Soori, 2021). Single decision trees can have high variance, whereas RF reduces variance by aggregating many trees (Casarin et al., 2021).

SVM performance depends strongly on kernel choice and tuning (Sajid, Muhammad, et al., 2021). Gradient-boosting methods were outside the scope of this study; their omission should not be interpreted as evidence that they necessarily overfit.

ML algorithms differ in their ability to represent linear and nonlinear decision boundaries (Suzuki et al., 2019). The linear SVM performed competitively in several datasets, whereas the radial-kernel SVM performed well in Datasets 7 and 8. This pattern may indicate nonlinear structure, but it is not a diagnostic test for nonlinearity. LR can also represent nonlinear effects when suitable transformations, splines, or interactions are specified. Similarly, SVM and RF are not inherently immune to outliers; their sensitivity depends on preprocessing, hyperparameters, and the data-generating process (Sajid, Muhammad, et al., 2021).

RF produced the highest cross-validation values in most datasets. Plausible explanations include its ability to represent interactions and nonlinearities and the variance reduction achieved by aggregating decorrelated trees (Liu et al., 2012; Rigatti, 2017). However, the present analysis did not isolate the mechanism responsible for RF's performance. In particular, low R^2 values in the original PLS-SEM models do not demonstrate nonlinearity. The results therefore support the empirical performance of RF in these datasets, not a general causal explanation for that performance.

For applications with binary endogenous outcomes, researchers may consider RF or radial-kernel SVM as predictive extensions to a PLS-SEM workflow, but model choice should be based on prespecified tuning and genuinely out-of-sample validation. Larger samples would permit more stable performance estimates and more reliable hyperparameter selection (Sajid, Almehmadi, et al., 2021). Reporting repeated resampling distributions or confidence intervals would further clarify the uncertainty in differences between algorithms.

This study has several limitations. First, the outcomes were created by dichotomizing continuous latent scores rather than observed as naturally binary endpoints. Dichotomization discards information and may alter both associations and predictive performance. Second, the smallest datasets produced very small test sets and unstable estimates. Third, the manuscript reports point estimates from several validation schemes but does not report repeated-resampling uncertainty or formal paired comparisons. Fourth, details of preprocessing, hyperparameter grids, class-balance handling, random seeds, and whether feature construction occurred entirely within each resampling loop require fuller reporting for reproducibility. Finally, the eight datasets do not establish that the observed ranking will generalize to other domains.

5. Conclusion

This study shows how PLS-SEM latent scores can be combined with supervised classifiers when the focal endogenous outcome is binary. Across eight secondary datasets, RF most frequently produced the highest cross-validation metrics, while radial-kernel SVM was competitive in some train-test evaluations. The advantage over LR was not uniform across datasets or validation designs, particularly in small held-out samples. These findings support comparing several prespecified classifiers under rigorous out-of-sample validation; they do not justify replacing LR automatically. Future studies should evaluate naturally binary outcomes, repeat resampling to quantify uncertainty, and report complete preprocessing and tuning procedures.

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