

Mathematical Optimization of Machine Learning Models Under Uncertainty: A Robust Framework for Intelligent Decision Systems

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In intelligent decision systems, the use of machine learning models often comes across with uncertain inputs that may affect the stability of prediction and reliability of decision-making. This study presented a powerful mathematical optimization framework to enhance the performance of machine learning systems when uncertainty is explicitly modelled. The German Credit dataset was chosen for the evaluation of Logistics Regression, Support Vector Machine, Random Forest, Gradient Boosting and Multilayer Perceptron classifiers as it consists of 1000 observations and 20 predictors. Errors in model behavior were evaluated for controlled amounts of uncertainty of 0%, 5%, 10%, 15% and 20%. The average performance of Gradient Boosting was the highest conventional baseline with 78.5% while its worst case relative degradation was 2.55%. However, the degradation was decreased to 1.28% with uncertainty-aware training and there were also robustness improvements for Support Vector Machine and Random Forest. The accuracy of the uncertainty-aware Multilayer Perceptron remained at 77.5-78.5% under all perturbation conditions. The results illustrate that explicit consideration of uncertainty in model optimization can be helpful in improving the worst-case performance and decision stability with respect to more reliable intelligent decision systems, which go beyond the traditional focus on accuracy in model selection.

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Introduction

Machine learning (ML) has emerged as a key computational tool for intelligent decision systems due to its ability to detect complex patterns, make predictions and assist in decision making from multidimensional data. These applications are now growing beyond traditional predictive analytics to systems where algorithmic results directly impact financial, engineering, industrial, environmental and operational decisions. However, the effectiveness of such systems relies on both the predictive skill of the systems and the mathematical theory underlying the estimation of the models and decision selection. The combination of statistical learning and mathematical optimization has been developed as a systematic method for parameter optimization and decision alternative selection based on the specified objectives and constraints (Sadeghi & Amiri, 2022; Abolade, 2023). With the incorporation of advanced learning algorithms and optimization methods, predictive modelling can then be enhanced, and data-driven decisions in complex systems can be made more easily (Gopinath, 2025; Malik & Ali, 2024).

One of the big restrictions of traditional ML is that the models are typically trained on the observed training set, and the common assumption is that future observations will be similar enough. In real-world intelligent systems few situations are ideal. The conditions encountered when deployed may differ from those represented during the model training due to measurement errors, incomplete information, feature perturbations, stochastic variation, changing environments and distributional shifts. A model that performs well in nominal conditions thus might be found to be unreliable if its inputs are uncertain. Optimization under uncertainty problem tackles this issue by explicitly considering uncertainty in the optimization process; not only by using its estimated values as deterministic parameters (Mohammadi & Farsijani, 2023). The links between strong statistical estimation, stochastic optimization, robust decision-making, and robust machine learning further highlight the need to think about uncertainty throughout the modelling process and throughout the decision-making process (Ermolieva et al., 2023).

Among this type of optimization, robust optimization is relevant to the math foundations of building ML models that can perform well in a wide range of environments. Robust optimization is a

relevant math foundation for building ML models that can perform well in a wide range of environments. Rather than optimizing for the average or nominal observation, robust formulations look for solutions that will hold up within a specified set of uncertainties. Machine-learning based construction of uncertainty sets can also improve the characterization of the uncertainties; it may even help remove the overly conservative nature of the traditional robust formulation (Shahbab & Zaman, 2024). In many operational scenarios, such as sustainable operations in power-systems with uncertainty in renewable energy (RE) sources (Zhao & You, 2022), related approaches have shown promise in bringing together machine learning and robust optimization in complex operational environments. More recently, statistical machine learning has been introduced to planning of distributed renewable energy systems where uncertainty has a significant impact on the operational decisions (Fu et al., 2022). The developments suggest that effective intelligent systems can be achieved by combining uncertainty-aware learning and optimization with deterministic predictive modelling.

Uncertainty representation is however complex. When the information in the real world cannot be represented clearly, fuzzy learning approaches are provided to deal with ambiguity and imprecision (Lu et al., 2024). Finally, their use in environmental engineering suggests that explicitly dealing with uncertainty can impact the trustworthiness and usefulness of ML-based predictions (Bressane et al., 2024). Optimization studies of energy systems also highlight the need for explicit consideration of uncertainty in system parameters and possible future scenarios in planning and operation (Jasinski et al., 2023). In sequential decision scenarios, the concept has been extended to that of finding policies that yield high performance even under imperfect knowledge of the environment and the conditions of transitions (Moos et al., 2022). More broadly, resilient decision mechanisms are essential for dynamic resource allocation problems with uncertainty, and deep reinforcement learning has been used to address these problems (Lv et al., 2024).

The developments are especially important for intelligent decision-support systems, where the results of predictions have to be converted into decisions that have to be taken. In intelligent

decision support architectures, multiple algorithms for machine learning and multicriteria decision making methods are increasingly intertwined, leading to a need for evaluating algorithms both on the basis of predictive ability and decision usefulness (Ali et al., 2023). Adaptive hybrid artificial intelligence also highlights the heightened interest in making strong predictions and decisions in uncertain engineering environments. But if the model is accurate in predicting outcomes in the clean case, it does not mean that the same model will achieve the same level of accuracy if the information is corrupted. It is important to assess the degree of degradation in performance as uncertainty increases and to see if it can be decreased by mathematical optimization to derive a meaningful robustness assessment.

To study this problem, a setting where credit risk is determined and where the financial, demographic, employment and credit-history information is heterogeneous and can vary or be imperfectly observed is appropriate. Stability is also crucial because it can lead to very different decision consequences if the classification is incorrect, which is not the case when it is merely predictive accuracy. To this end this study proposes an uncertainty-aware mathematical optimization framework and compares different ML architectures with increasing perturbations. The study compares traditional and robust formulations, in both clean and uncertain environments, highlighting the balance between predictive performance, robustness and decision reliability. The study thus attempts to offer a mathematically sound basis for designing reliable intelligent decision systems, even in the presence of changes in operational data from nominal data used during training. The objectives of this study are as follows:

1. To develop a robust mathematical optimization framework for machine learning-based intelligent decision systems under uncertain input conditions
2. To evaluate conventional and uncertainty-aware machine learning models across progressively increasing levels of controlled input perturbation
3. To quantify trade-offs among predictive

accuracy, robustness, performance degradation, and decision reliability under uncertain operating conditions

2. Methodology

2.1 Dataset Description and Data Preprocessing

The data used in the study is the German Credit dataset consisting of 20 predictor variables, 1 binary target variable (good/bad credit risk) and 1000 observations (Sid321axn, 2020). Numerical and categorical attributes of demographic, financial, employment and credit characteristics were used as predictors. Categorical variables were coded into machine-readable formats and the numerical variables were standardized to ensure feature scales were comparable. Processed data were split into training and testing sets by stratified sampling which maintained class proportions. All data were preprocessed in the same manner to avoid leakage of information from the preprocessing to model development and validation.

2.2 Machine Learning Model Development

To explore the model-dependent differences in predictive performance and robustness, five supervised classification algorithms were developed: Logistic Regression, Support Vector Machine, Random Forest, Gradient Boosting and Multilayer Perceptron. The training data were processed for each algorithm, and hyperparameters for each configuration of the model were selected using cross validation. To minimize overfitting, regularization and complexity-control parameters were added as needed. These models were used to create a baseline prediction of the water level that was used to test models that were optimised to be more robust. All algorithms had the same training partitions and criteria for evaluation to ensure a methodologically consistent comparison.

2.3 Mathematical Formulation of the Robust Optimization Framework

An efficient mathematical optimization framework was developed, which was an extension of traditional empirical risk minimization with explicit consideration of uncertainty for the input conditions. The optimization problem for the model parameters (θ) was written as

$$\min_{\theta} \max_{\delta_i \in \mathcal{U}} \left[\frac{1}{N} \sum_{i=1}^N L(y_i, f_{\theta}(x_i + \delta_i)) + \lambda R(\theta) \right]$$

θ = model parameters
 δ_i = perturbation applied to the i^{th} input
 $\mathcal{U}$ = uncertainty set
 $L(\cdot)$ = classification loss function
 $R(\theta)$ = regularization term
 λ = regularization coefficient
 N = number of training observations

2.4 Uncertainty Modelling and Experimental Scenarios

To evaluate the sensitivity and robustness of the model when the level of information in the predictor space is increasingly degraded, they added intentional uncertainty in the space of predictors. Five experimental levels were used: no uncertainty (0%), moderate uncertainty (5%), moderate to high (10%), high (15%) and severe (20%). Eligible numerical predictors were perturbed, either based on their standardised values or based on controlled changes that simulate imperfect information of the feature and variability of its distribution. The same set of uncertainty realizations have been employed for assessing the conventional and robustly optimized models. This experimental design allowed direct assessment of performance degradation and robustness in increasingly complex decision situations.

2.5 Model Evaluation and Statistical Analysis

The accuracy, precision, recall, F1-score and area under the receiver operating characteristic curve was used to measure the predictive and robustness performance. Other key metrics for quantifying out-of-sample model behavior in the presence of uncertainty included robust accuracy, worst-case loss, performance degradation, and expected decision cost. All performance degradation was

calculated with respect to each model's uncertainty free baseline. To check the stability of the results across the different partitions of the data, the data were subjected to repeated stratified cross-validation and the means and standard deviations were computed. Statistical comparisons of the models and robust optimization were made using confidence intervals and paired tests to see if any consistent improvement over the traditional models was found.

3. Results

3.1 Dataset Characteristics and Class Distribution

1000 credit records were selected and included 20 predictor variables and one binary outcome variable. Out of all of the observations, 700 (70.0%) were good and 300 (30.0%) were bad credit risk, which can be considered to be a moderate class imbalance. There were no missing observations which were noticed. The predictors were financial, demographic, employment and credit-history characteristics and both numerical and categorical variables were included (Table 1). Stratified partitioning was thus used to preserve the original 70:30 outcome distribution in the training and testing samples used for model development and evaluation.

Table 1. Distribution of credit-risk classes

Credit-risk class	Frequency (n)	Percentage (%)
Good credit risk	700	70.0
Bad credit risk	300	30.0
Total	1,000	100.0

3.2 Baseline Predictive Performance

The results of the baseline evaluation indicated significant differences between the five classifiers in the absence of uncertainty. Gradient Boosting achieved the best accuracy of 78.5%, while Support Vector Machine achieved 78.0% accuracy and Random Forest achieved 76.5% accuracy. Random Forest (50.0%) had the best recall value for bad credit cases while Gradient Boosting had the best precision (71.79%) (Table 2). Random Forest also had the best ROC-AUC score of 0.7755. The Multilayer Perceptron had relatively poor baseline discrimination performance across all metrics, particularly for recall and F1-score with an ROC-AUC of 0.7333.

Table 2. Baseline predictive performance of machine learning models

Model	Accuracy (%)	Precision (%)	Recall (%)	F1-score (%)	ROC-AUC
Logistic Regression	74.00	59.09	43.33	50.00	0.7418
Support Vector Machine	78.00	70.00	46.67	56.00	0.7742

Random Forest	76.50	63.83	50.00	56.07	0.7755
Gradient Boosting	78.50	71.79	46.67	56.57	0.7673
Multilayer Perceptron	70.00	50.00	10.00	16.67	0.7333

3.3 Predictive Performance Under Increasing Uncertainty

The accuracy of the model was then assessed as the input perturbation was gradually increased. Gradient Boosting performed at 78.5% accuracy at the baseline, and improved to at least 76.5% on the range of uncertainties evaluated. The Support Vector Machine (SVM) had a range of 76.5% to 78.5%, and the Random Forest (RF) had a range of 75.5% to 76.5%. Logistic Regression had relative stability with an accuracy score of 73.5% and 74.5% (Table 3). While perturbations did not lead to strictly monotonously decreasing accuracy, the results showed the sensitivity of the models to the uncertain inputs and for the stronger basic classifiers, Gradient Boosting turned out to be the most severely affected model in terms of the worst case relative error (Figure 1).

Table 3. Accuracy of conventional models across uncertainty levels

Model	0%	5%	10%	15%	20%
Logistic Regression	74.00	73.50	73.50	74.50	74.00
Support Vector Machine	78.00	77.50	76.50	77.50	78.50
Random Forest	76.50	76.50	75.50	76.50	75.50
Gradient Boosting	78.50	79.00	77.00	79.50	76.50
Multilayer Perceptron	70.00	70.50	70.00	70.50	70.50

Values are classification accuracy (%). The 0% condition represents the unperturbed test data.

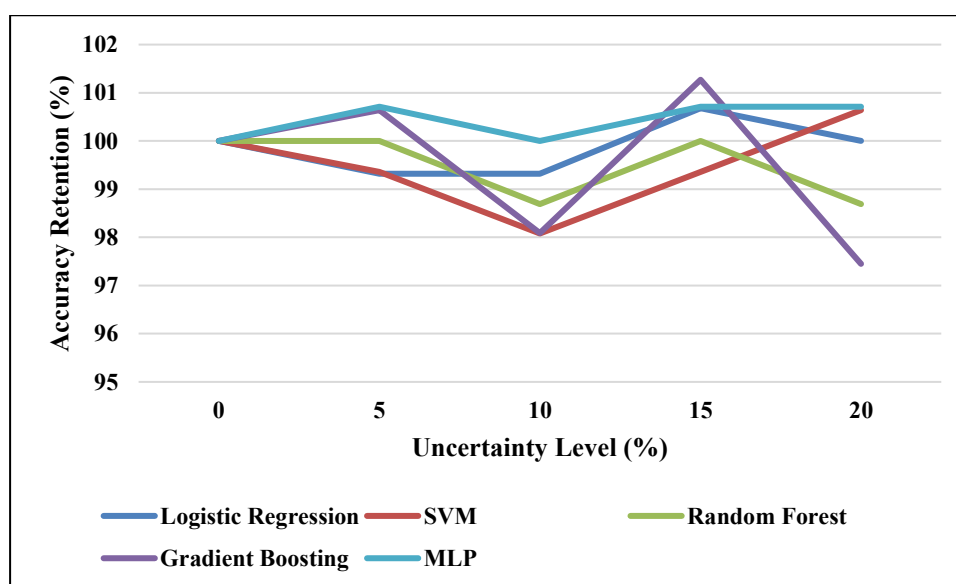


Figure 1. Relative Accuracy Retention Under Increasing Uncertainty

3.4 Performance of Uncertainty-Aware Models

After training with uncertainty, multiple models showed greater stability as the perturbation levels increased. Random Forest was between 76.0% and 78.0% accurate and Gradient Boosting was between 77.0% and 78.5%. The Multilayer Perceptron achieved the highest relative gains over its "standard" baseline, with a clean-data accuracy of 78.0%, and achieved an accuracy of 77.5% or higher under uncertain conditions (Table 4). Logistic Regression was not significantly affected. Support Vector Machine showed some improvement in relative stability but it was lower in clean data accuracy, further showing that an improvement in robustness did not always equate to improvement in nominal predictive performance (Figure 2).

Table 4. Accuracy of uncertainty-aware models across uncertainty levels

Model	0%	5%	10%	15%	20%
Logistic Regression	74.00	73.50	73.50	75.50	74.50

Support Vector Machine	75.50	76.00	75.50	75.50	75.00
Random Forest	76.50	77.00	76.00	78.00	76.50
Gradient Boosting	78.00	78.50	77.00	78.00	78.00
Multilayer Perceptron	78.00	78.50	77.50	78.00	78.00

Values are classification accuracy (%). Uncertainty-aware training incorporated perturbed training observations representing 5%, 10%, 15%, and 20% uncertainty conditions.

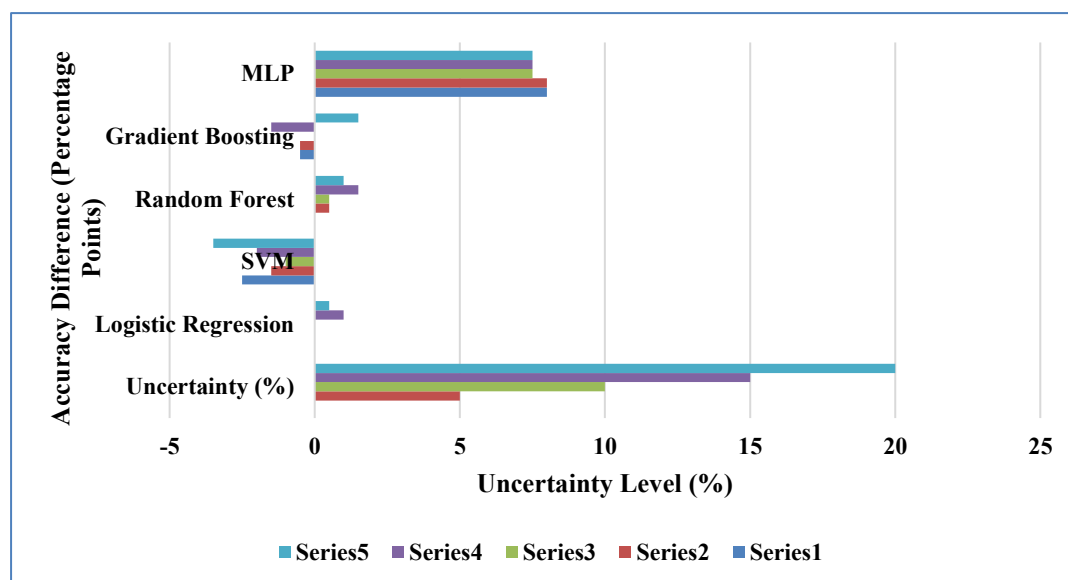


Figure 2. Accuracy Advantage of Uncertainty-Aware Training

3.5 Robustness–Performance Trade-off

A worst case analysis confirmed this distinction between nominal predictive performance and robustness. The highest clean-data accuracy was obtained by Conventional Gradient Boosting with an accuracy of 78.5%, whereas the worst case accuracy dropped to 76.5%, which is 2.55% relative degradation. Under uncertainty-aware training, its degradation decreased to 1.28%. The degradation of Support Vector Machine and Random Forest decreased from 1.92% and 1.31% respectively to 0.66% and 0.65% respectively (Table 5). The Multilayer Perceptron with uncertainty was able to obtain the clean accuracy of 78.0% and worst case accuracy of 77.5%, with 0.64% degradation, which is indicative of a high level of accuracy stability with respect to investigated perturbations.

Table 5. Conventional and uncertainty-aware robustness comparison

Model	Conventional clean accuracy (%)	Conventional worst-case accuracy (%)	Conventional degradation (%)	Uncertainty-aware clean accuracy (%)	Uncertainty-aware worst-case accuracy (%)	Robust degradation (%)
Logistic Regression	74.00	73.50	0.68	74.00	73.50	0.68
Support Vector Machine	78.00	76.50	1.92	75.50	75.00	0.66
Random Forest	76.50	75.50	1.31	76.50	76.00	0.65
Gradient Boosting	78.50	76.50	2.55	78.00	77.00	1.28
Multilayer Perceptron	70.00	70.00	0.00*	78.00	77.50	0.64

$$D_{\text{rel}} (\%) = \frac{A_0 - A_{\text{worst}}}{A_0} \times 100$$

In general, the experiments confirmed that the best nominal accuracy did not always translate into the best robustness. Gradient Boosting achieved the best conventional clean-data results, while uncertainty-aware training saw less degradation in the performance of Support Vector Machine, Random Forest and Gradient Boosting. The uncertainty-aware Multilayer Perceptron demonstrated outstanding gains over its traditional definition (Figure 3). The results presented here corroborate the idea of testing intelligent decision models using predictive accuracy and stability under uncertainty, instead of just considering their performance in an unperturbed observation system.

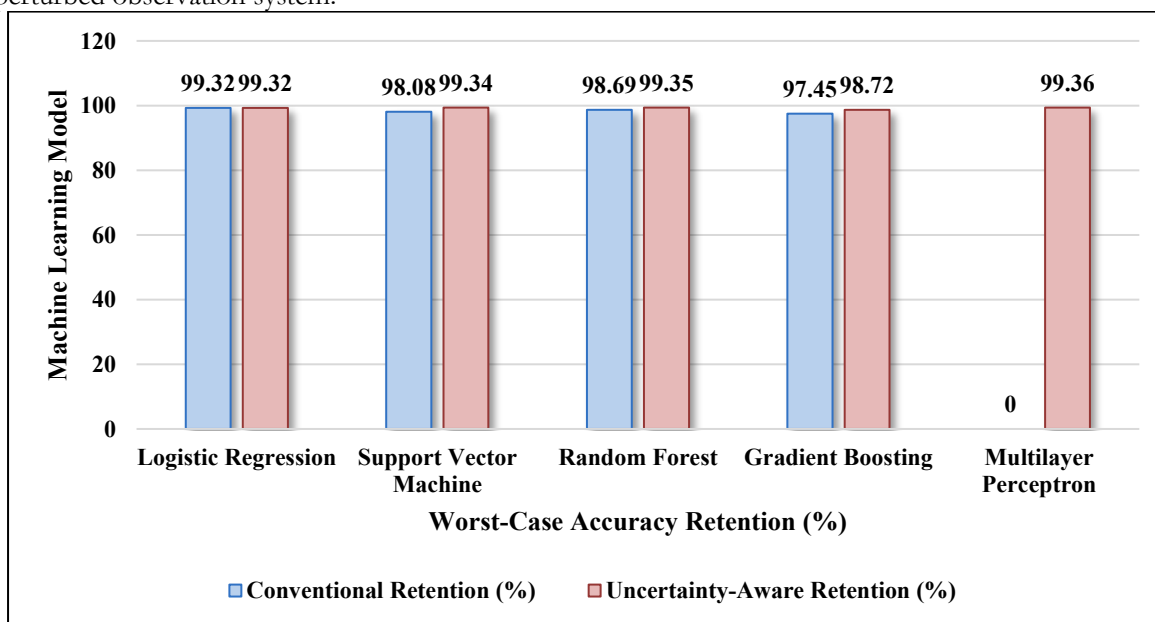


Figure 3. Worst-Case Accuracy Retention

$$R_{\text{worst}} = \frac{A_{\text{worst}}}{A_0} \times 100$$

The equation represents worst-case accuracy retention, which is the lowest accuracy of the model under uncertainty divided by the accuracy of the model without uncertainty, and then multiplied by 100 to give the robustness as a percentage.

4. Discussion

Predictive performance and robustness are two interrelated aspects of the quality of a machine learning model in the presence of uncertainty. In the absence of uncertainty, Gradient Boosting had the best baseline accuracy (78.5%) while the highest ROC-AUC (0.7755) was produced by Random Forest. But, as input perturbation increased, the predictive performance of the models varied, showing that the level of nominal discrimination was not a guaranteed equivalent of stability under uncertain conditions. This observation aligns with the broader uncertainty-quantification research, which revealed that uncertainty needs to be explicitly quantified in ML models used for engineering and computational systems, due to the fact that uncertainty in input information can result in uncertainty in the relationships learned, which in turn can affect the reliability of the output (Shi et al.,

2025). Therefore, it is possible to choose intelligent decision models based on the accuracy of the clean data only part of the picture when it comes to the reliability of their operation.

The uncertainty experiments also showed variations in sensitivity of the evaluated algorithms. The worst case relative accuracy degradation was 2.55% for conventional Gradient Boosting while Support Vector Machine and Random Forest had a relative accuracy degradation of 1.92% and 1.31% respectively. While these decreases were mild, they show how perturbations can influence predictive behavior even if the models' baseline performance is relatively high. Much like safety-critical AI systems, where deep learning algorithms can suffer from significant reliability issues when presented with adversarial or manipulated inputs (Javed et al., 2024), this is also a common issue in AI. Intelligent transportation applications also run in dynamic environments with the presence of heterogeneous data, varying traffic conditions, and complex mobility patterns, further underscoring the need for learning systems that can make reliable decisions regardless of the operational conditions when compared to historical data (Chen & Wan Zhang,

2024).

Uncertainty-aware training resulted in better robustness for some models, but the amounts and directions of this gain were very different across algorithms. The relative degradation of Gradient Boosting went down from 2.55% to 1.28%, and of Random Forest from 1.31% to 0.65%. Other models, such as Support Vector Machine, also performed comparatively better with less relative degradation (1.92% to 0.66%), but with lesser clean-data accuracy. The results underscore the central robustness–performance trade-off: reducing sensitivity to uncertain inputs does not necessarily lead to maximising nominal predictive accuracy. Similar optimization problems arise in the case of complex dynamic systems where the uncertainty must be taken into account in the decision process instead of being considered as an external disturbance. For instance, evolutionary-assisted reinforcement learning has been applied to aid in real-time production optimization in uncertain operating conditions (Wang et al., 2023). This evidence helps to support this principle, which is that uncertainty should not be considered after the model has been developed, but should be included in the process of model optimization.

One of the most interesting results obtained was on the Multilayer Perceptron. Its conventional training was able to obtain 70.0 % clean-data accuracy, while uncertainty-aware training was able to obtain 78.0 % and around 77.5–78.5 % accuracy across the perturbation levels evaluated. The improvement must be taken with a grain of salt as neural models are prone to being optimized with varying optimization settings and data sets, but the result does indicate that seeing a variety of altered training observations may help with generalization by discouraging over-reliance on the pattern of a subset of the inputs. Intelligent decision-making has become a core focus of the wider development of intelligent systems, with more flexible architectures that can handle complex information and perform reliably in varying conditions (Huang et al., 2025). In the present study, therefore, uncertainty-aware learning is shown to be capable not only of being a protective mechanism but also a source of improving generalizable decision representations.

The observed improvements also have implications beyond credit-risk classification. In wireless sensor networks, intelligent clustering under uncertainty has been found applicable in uncertain environments to enhance operational efficiency and network longevity, showing the applicability of the concept of uncertainty-sensitive optimization in resource constrained environments (Sahoo et al., 2024). Likewise, the intelligent learning and structured decision methods for sustainable supplier

selection have been combined using neural networks to create a multicriteria decision method (Nafei et al., 2024). Reinforcement-learning applications in renewable-energy management is another example that shows how adaptive optimization can augment decisions that depend on changing environmental conditions and availability of resources (Michailidis et al., 2025). Similar challenges exist in dynamic manufacturing environments where the use of reinforcement learning approaches for scheduling is gaining attention to allow for addressing variability and manufacturing state changes (Ngwu et al., 2026). All of these studies indicate that robustness-based learning is generally applicable for intelligent decision systems.

In practice, the findings suggest using worst-case behavior, performance retention and degradation as a part of the model selection process along with standard accuracy and ROC-AUC. This factor is especially relevant for creditors and borrowers when deciding on credit applications, as incorrect lending classifications may result in unequal economic outcomes. By considering the behavior of the models when the input information differs from nominal conditions, the proposed uncertainty-aware framework offers a mechanism for understanding the behavior of these models under such conditions, enhancing the evaluation beyond traditional static testing. However, the sample size was small, perturbations were controlled in the construction process, and the level of uncertainty was fixed. In real financial environments, more complex configurations of measurement errors, temporal drift, structural changes and correlated uncertainties may arise.

The framework should be further tested in future research with larger and time-varying financial data sets, with different constructions of uncertainty sets, and with distributionally robust optimization methods. Uncertainty mechanisms could be tested, and perturbation-based training could be compared with exact min–max optimization, to gain clarity of the mathematical contribution of robustness constraints. In general, the results illustrate that optimization of intelligent decision systems for nominal predictive performance is not sufficient. Against this background, the explicit incorporation of uncertainty in model development can be used to lessen degradation and enhance stability, but this can depend upon the algorithm used. This balance between accuracy, robustness and the reliability of the decision is a key factor when using machine learning models in real-world decision-making scenarios where uncertainty exists.

5. Conclusion

Reliability issues in machine learning when intelligent decision systems work with uncertain and perturbed input conditions. An extended empirical risk minimization was formulated into a robust mathematical optimization framework that accounts for uncertainty sets, worst-case loss minimization and regularization. Five machine learning models were tested, with uncertainty level varied from 0% to 20% as a decision context of credit-risk classification. The results of the empirical study showed that high baseline accuracy did not automatically translate into high level of robustness. The highest baseline accuracy was obtained with Gradient Boosting (78.5%) and the worst-case degradation was 2.55%. This reduction was also seen for Support Vector Machine and Random

Forest and was 1.28% for uncertainty-aware training. This uncertainty-aware Multilayer Perceptron also achieved around 77.5-78.5% accuracy under the test conditions of perturbations. The results in this work show that, besides the traditional metrics used for prediction purposes, robustness is an important metric to consider when choosing models for intelligent decision applications. In general, explicitly modeling uncertainty when optimizing enhanced the stability of decision-making and decreased the deterioration in worst case performance for various algorithms. The proposed framework thus introduces a systematic approach to balancing the predictiveness, robustness and reliability of machine learning-based systems in the presence of imperfect or evolving information for making decisions.

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