



Uncertainty-Aware Feature Selection Framework Based on Three-Way Decision Theory for Explainable Machine Learning

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Abstract: Feature selection is a critical stage in machine learning because it improves predictive performance, reduces computational complexity, and enhances model interpretability. However, many existing feature selection methods rely on binary selection strategies that either retain or discard features based on fixed relevance thresholds. This approach can be inadequate when features contain uncertainty, instability, redundancy, or borderline predictive value. To address this limitation, this article proposes an uncertainty-aware feature selection framework based on three-way decision theory for explainable machine learning. The proposed framework classifies features into three decision regions: accepted features, rejected features, and deferred features. Accepted features are considered highly relevant and reliable, rejected features are removed due to low relevance or high redundancy, while deferred features are subjected to further evaluation because of uncertain or inconsistent importance. By integrating uncertainty measurement with feature relevance scoring, the framework provides a more flexible and transparent alternative to conventional two-way feature selection. The framework also supports explainability by providing clear justification for why each feature is selected, rejected, or deferred. This makes it particularly useful for high-dimensional and high-stakes machine learning applications where model transparency, reliability, and decision accountability are important. The proposed approach is expected to improve feature selection stability, reduce uncertainty in selected feature subsets, and enhance the interpretability of machine learning models.

Keywords: Three-Way Decision Theory, Uncertainty-Aware Feature Selection, Explainable Machine Learning, Feature Relevance, Feature Uncertainty, Rough Set Theory, Model Interpretability, Decision-Theoretic Learning.

1. Introduction

Feature selection remains a central component of machine learning pipelines due to its ability to reduce dimensionality, improve predictive accuracy, and enhance model interpretability. In many real-world applications such as healthcare diagnosis, cybersecurity, and financial risk modeling, datasets often contain high-dimensional and noisy attributes that complicate learning processes. Conventional feature selection methods typically rely on deterministic or binary decision rules in which features are either selected or discarded based on fixed thresholds or ranking scores. While effective in structured environments, such approaches struggle when feature relevance is uncertain, unstable, or context dependent.

Uncertainty is a persistent challenge in modern machine learning systems. It arises from incomplete data, noise, overlapping class distributions, and variability in model estimation. In such cases, forcing a strict inclusion or exclusion decision may lead to the loss of potentially useful information or the retention of misleading features. This limitation becomes more critical in high-stakes environments where interpretability and decision reliability are essential. Research has shown that ignoring uncertainty in predictive modeling can significantly reduce robustness and

trustworthiness in deployment settings (Hüllermeier & Waegeman, 2021).

Explainable machine learning has emerged as a response to the growing need for transparency in algorithmic decision-making. However, much of the existing work in explainability focuses on post-hoc interpretation of black-box models rather than integrating interpretability into the feature selection process itself. This creates a gap between feature selection and explainability, where selected features may still lack clear justification for their inclusion. Studies have emphasized the importance of inherently interpretable approaches that provide transparent reasoning throughout the modeling pipeline rather than after training (Rudin, 2019).

To address these limitations, uncertainty-aware learning frameworks have gained increasing attention. In particular, three-way decision theory offers a structured mechanism for handling uncertainty by introducing a third decision region in addition to traditional acceptance and rejection classes. This intermediate region allows ambiguous cases to be deferred for further analysis instead of being prematurely categorized. Such a mechanism aligns naturally with feature selection problems, where some attributes cannot be confidently classified as either relevant or irrelevant.

This study proposes an uncertainty-aware feature selection framework based on three-way decision theory for explainable machine learning. The framework introduces a structured process that categorizes features into accepted, rejected, and deferred groups based on both relevance and uncertainty measures. By integrating uncertainty modeling with decision-theoretic reasoning, the framework aims to improve feature selection stability, reduce information loss, and strengthen interpretability in machine learning models.

The main objective of this work is to develop a transparent and adaptive feature selection mechanism that supports explainable artificial intelligence systems in complex data environments. The proposed approach contributes to bridging the gap between uncertainty handling and explainable feature selection by embedding decision transparency directly into the feature evaluation process.

2. Literature Review

2.1. Feature Selection in Machine Learning

Feature selection is a fundamental preprocessing step in machine learning that aims to identify the most informative subset of features while discarding irrelevant or redundant ones. It improves model performance, reduces computational cost, and enhances interpretability. Classical feature selection methods are generally grouped into filter, wrapper, and embedded approaches. Filter methods rely on statistical measures such as correlation and mutual information, wrapper methods evaluate feature subsets using predictive performance, while embedded methods integrate feature selection directly into model training.

Despite their wide adoption, these methods often assume that feature relevance is deterministic and clearly separable. This assumption becomes problematic in high-dimensional and noisy datasets where feature importance is unstable or context dependent. As a result, feature selection outcomes may vary significantly across different samples or model configurations, reducing reliability in practical applications.

2.2. Limitations of Conventional Feature Selection Methods

Conventional feature selection techniques are largely based on binary or ranked decision strategies. A feature is either selected or discarded based on a threshold or importance score. This rigid structure does not adequately capture borderline cases where a feature may exhibit partial relevance or context-dependent usefulness.

Another limitation is the sensitivity of these methods to data distribution shifts and noise. Small perturbations in training data can lead to different feature rankings, which undermines stability. Furthermore, most traditional approaches do not explicitly represent uncertainty in feature evaluation, leading to overconfident decisions even in ambiguous conditions.

2.3. Uncertainty in Machine Learning

Uncertainty is an inherent characteristic of real-world machine learning systems. It is commonly categorized into

aleatoric uncertainty, which originates from noise in the data, and epistemic uncertainty, which arises from incomplete knowledge or limited data coverage. Both forms of uncertainty directly influence feature relevance estimation and model predictions.

Hüllermeier and Waegeman (2021) emphasize that proper uncertainty modeling is essential for building reliable machine learning systems, particularly in domains where incorrect decisions carry significant consequences. Ignoring uncertainty may result in unstable models and misleading interpretations, especially in high-dimensional feature spaces.

2.4. Three-Way Decision Theory

Three-way decision theory extends classical decision-making frameworks by introducing a third option in addition to acceptance and rejection. This third region, often referred to as the boundary or deferment region, allows uncertain cases to be postponed for further evaluation rather than being forcefully classified.

This structure is particularly useful in environments where information is incomplete or ambiguous. In feature selection, it provides a principled way to handle features that cannot be confidently classified as either relevant or irrelevant. Instead of forcing a binary decision, such features can be temporarily deferred for additional analysis, reducing the risk of incorrect elimination.

2.5. Rough Sets and Feature Evaluation

Rough set theory provides a mathematical foundation for reasoning under uncertainty without requiring probabilistic assumptions. It defines lower and upper approximations to represent certain and possible memberships within a dataset. In feature selection, rough sets are used to evaluate attribute dependency and significance based on data granularity.

When combined with three-way decision theory, rough sets enable a more flexible representation of feature relevance. Features located in boundary regions can be explicitly modeled rather than ignored or forced into binary categories. This improves robustness in uncertain environments and supports more informed feature selection decisions.

Liu et al. (2026) highlight that rough feature selection methods remain highly relevant in modern high-dimensional learning tasks, particularly where uncertainty and incomplete information are prevalent.

2.6. Explainable Machine Learning and Feature Selection

Explainable machine learning focuses on making model decisions transparent and understandable to human users. While post-hoc explanation techniques such as SHAP and LIME are widely used, they do not influence the feature selection process itself. This creates a gap between model interpretability and feature selection transparency.

Rudin (2019) argues that interpretability should be built into machine learning models rather than added after training. In this context, feature selection plays a critical role because selected features directly determine how predictions are generated and interpreted. However, most traditional feature selection methods do not provide explicit reasoning for why a feature is selected or rejected.

2.7. Research Gap

Despite significant advances in feature selection, uncertainty modeling, and explainable artificial intelligence, these areas remain largely disconnected in practice. Existing feature selection techniques rarely incorporate structured uncertainty handling mechanisms that allow ambiguous features to be treated differently from clearly relevant or irrelevant ones.

Furthermore, explainable AI methods often focus on interpreting model outputs rather than explaining the feature selection process itself. This creates a transparency gap in early-stage decision-making within machine learning pipelines. There is also limited integration of three-way decision theory into feature selection frameworks for explainability purposes, despite its strong theoretical suitability for handling uncertainty.

This study addresses this gap by proposing an uncertainty-aware feature selection framework based on three-way decision theory. The framework explicitly models acceptance, rejection, and deferment regions while integrating uncertainty quantification and interpretability into the feature selection process.

Table 1: Summary of Related Studies

Study / Author	Method	Uncertainty Handling	Explainability Support	Key Limitation
Arrieta et al. (2020)	XAI taxonomy and survey	Low	High	No feature selection integration
Rudin (2019)	Interpretable ML models	Moderate	High	Limited uncertainty modeling
Hüllermeier & Waegeman (2021)	Uncertainty framework	High	Low	Not feature-selection focused
Campagner et al. (2024)	Three-way decision ML review	High	Moderate	Limited practical feature frameworks
Liu et al. (2026)	Rough feature selection survey	High	Moderate	Weak integration with XAI
Alsakarnah et al. (2026)	Hybrid XAI feature selection	Moderate	High	Application-specific
Zschech et al. (2022)	Explainable feature selection	Moderate	High	Limited uncertainty modeling

3. Theoretical Foundation

3.1. Decision-Theoretic Basis of Three-Way Decisions

Three-way decision theory extends classical decision models by introducing a structured mechanism for handling uncertainty through three distinct regions: acceptance, rejection, and deferment. Unlike binary decision systems that force a strict yes or no outcome, this framework allows uncertain cases to remain undecided until sufficient evidence is available.

In decision-theoretic rough sets, each decision is associated with a cost structure that reflects the risk of incorrect classification. The optimal decision is then determined by minimizing expected loss under uncertainty. This principle provides a strong theoretical basis for feature selection, where each feature can be evaluated not only by its relevance but also by the cost of misclassification if it is incorrectly included or excluded.

In the context of feature selection, the acceptance region corresponds to features with strong predictive contribution, the rejection region contains irrelevant or noisy features, and the deferment region captures borderline features that require additional evaluation before a final decision is made. This structured decision mechanism provides a more realistic

representation of feature importance in uncertain environments (Campagner et al., 2024).

3.2. Feature Relevance and Redundancy

Feature relevance refers to the degree to which a feature contributes meaningful information toward predicting a target variable. However, relevance alone is not sufficient for feature selection because redundant features may carry overlapping information, reducing model efficiency without improving performance.

Redundancy arises when multiple features encode similar patterns or when a feature is strongly correlated with others. A robust feature selection framework must therefore balance relevance and redundancy while also considering uncertainty in feature contribution. This requires a scoring mechanism that evaluates not only individual feature strength but also its interaction with other features.

3.3. Uncertainty Measurement in Feature Selection

Uncertainty in feature evaluation arises when there is insufficient evidence to confidently determine whether a feature is relevant or irrelevant. This may result from noisy data, overlapping feature distributions, or unstable feature importance across different samples.

Common approaches to quantify uncertainty include entropy-based measures, variance in feature importance across resampling methods, and probabilistic confidence scores derived from predictive models. These measures provide a numerical representation of ambiguity in feature behavior, which can be incorporated into decision rules.

Hüllermeier and Waegeman (2021) emphasize that distinguishing between aleatoric and epistemic uncertainty is essential for reliable learning systems. In feature selection, epistemic uncertainty is particularly important because it reflects incomplete knowledge about feature behavior, which directly affects selection stability.

3.4. Explainability Through Feature Decision Reasoning

Explainability in feature selection requires that each decision is supported by a clear and interpretable

justification. Rather than simply identifying important features, an explainable system must explain why a feature was selected, rejected, or deferred.

In this framework, accepted features are those with high relevance and low uncertainty, rejected features exhibit low relevance or high redundancy, and deferred features represent ambiguous cases with conflicting or unstable signals. This structured reasoning enhances transparency and allows stakeholders to understand how input variables influence model construction.

Rudin (2019) argues that interpretability should be embedded directly into the modeling pipeline rather than applied after model training. This principle aligns with the integration of explainability into feature selection itself rather than treating it as a separate post-hoc process.

Theoretical Foundation of Uncertainty-Aware Three-Way Feature Selection

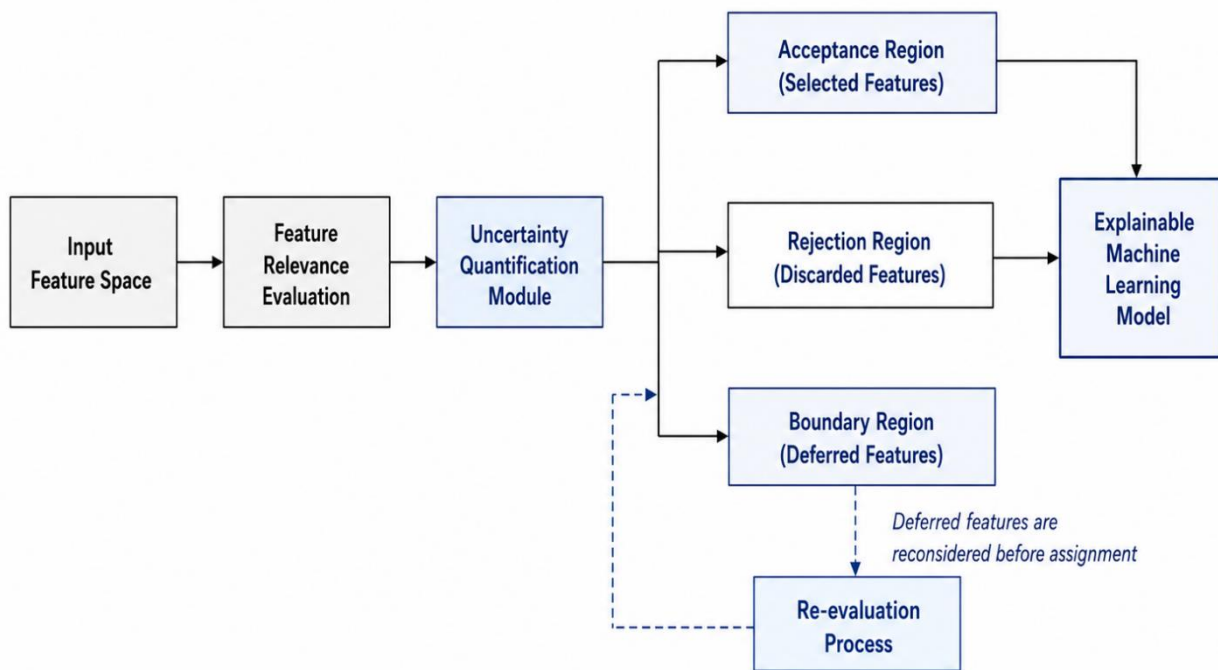


Fig 1: Uncertainty-Aware Three-Way Feature Selection Framework

4. Proposed Uncertainty-Aware Feature Selection Framework

4.1. Overview of the Framework

The proposed framework introduces an integrated mechanism for uncertainty-aware feature selection using three-way decision theory. The core idea is to move beyond binary feature selection by allowing features to be categorized into accepted, rejected, and deferred groups based on both relevance and uncertainty measurements.

The framework is designed to improve stability in high-dimensional learning environments while ensuring that feature selection decisions remain interpretable. It also supports iterative refinement of uncertain features through additional evaluation stages, making it suitable for complex and noisy datasets.

4.2. Data Preprocessing

The first stage involves preparing the dataset for analysis. This includes handling missing values through

imputation techniques, normalizing numerical attributes, encoding categorical variables, and removing extreme outliers where necessary.

Proper preprocessing ensures that feature relevance estimation is not biased by scale differences or data inconsistencies. It also improves the reliability of uncertainty estimation by reducing noise introduced by poor-quality data.

4.3. Feature Relevance Scoring

Each feature is assigned a relevance score that reflects its predictive contribution to the target variable. This score may be computed using statistical measures such as mutual information, correlation analysis, or model-based importance derived from ensemble methods.

The relevance score serves as the primary indicator of feature usefulness. However, it is not used in isolation. Instead, it is combined with uncertainty measures to determine the final decision region of each feature.

4.4. Uncertainty Estimation Mechanism

Uncertainty is estimated for each feature to capture instability in its predictive contribution. This may involve measuring variance in feature importance across cross-validation folds, entropy-based instability, or probabilistic confidence derived from multiple model runs.

Features with high variability in importance are considered uncertain, even if their average relevance is moderate. This prevents unstable features from being incorrectly selected and ensures that only reliable patterns are used in model construction.

4.5. Three-Way Decision Feature Partitioning

Once relevance and uncertainty scores are computed, features are classified into three regions:

- Acceptance Region: Features with high relevance and low uncertainty are selected for model training.
- Rejection Region: Features with low relevance or high redundancy are removed from the dataset.
- Boundary Region: Features with moderate relevance but high uncertainty are not immediately

decided and are passed to a secondary evaluation stage.

This structure prevents premature elimination of potentially useful features and improves decision robustness in uncertain environments.

4.6. Secondary Evaluation of Deferred Features

Features placed in the boundary region undergo additional evaluation to determine their final status. This may involve re-estimation of feature importance using alternative models, deeper statistical analysis, or expert validation in domain-specific applications.

This iterative process ensures that uncertain features are not permanently discarded without sufficient evidence. It also improves the overall stability of the feature selection process by reducing randomness in final feature subsets.

4.7. Explainability Layer

The explainability layer provides transparent reasoning for each feature decision. For every feature, the system records its relevance score, uncertainty level, and final decision category. This information is used to generate interpretable explanations that justify why a feature was selected, rejected, or deferred.

This layer enhances trust in the model by making feature selection decisions traceable and understandable. It also supports regulatory and domain-specific requirements where justification of model inputs is necessary.

4.8. Algorithmic Workflow of the Framework

The overall process of the framework can be summarized as follows:

1. Input dataset is preprocessed and normalized.
2. Feature relevance scores are computed.
3. Uncertainty values are estimated for each feature.
4. Three-way decision rules are applied.
5. Features are assigned to acceptance, rejection, or boundary regions.
6. Deferred features undergo secondary evaluation.
7. Final feature subset is passed to the machine learning model.
8. Explainability layer generates decision justification for all features.

Uncertainty-Aware Three-Way Decision Feature Selection Framework for Explainable Machine Learning

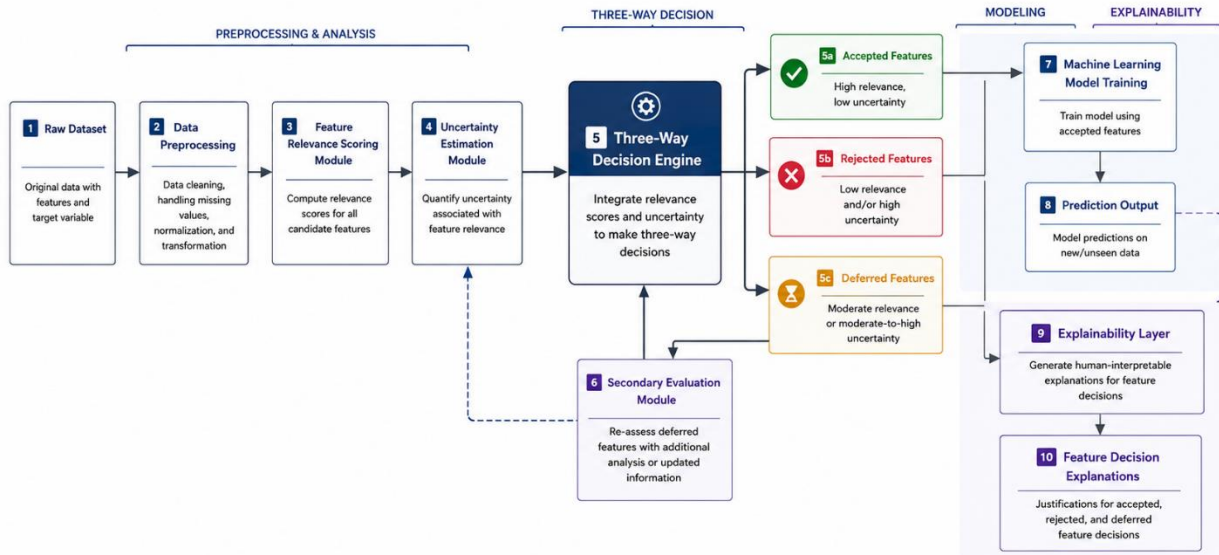


Fig 2: Uncertainty-Aware Three-Way Feature Selection Framework For Explainable Machine Learning

5. Methodology

5.1. Research Design

This study adopts an experimental machine learning research design to develop and evaluate an uncertainty-aware feature selection framework based on three-way decision theory. The methodology focuses on designing a feature selection process that does not rely only on binary inclusion or exclusion decisions. Instead, the proposed method classifies features into three decision regions: accepted, rejected, and deferred.

The experimental design is structured to evaluate the framework from three perspectives: predictive performance, uncertainty reduction, and explainability. This is necessary because a feature selection method should not only improve classification results but should also provide transparent justification for why specific features are selected or removed. This aligns with the broader argument that interpretability should be embedded within the learning

pipeline rather than added only after model training (Rudin, 2019).

5.2. Dataset Selection

The proposed framework is intended for evaluation using benchmark classification datasets with different levels of dimensionality, feature redundancy, and uncertainty. Suitable datasets may be selected from domains where explainability and reliable feature selection are important, such as healthcare, finance, cybersecurity, and bioinformatics.

The datasets should contain a mixture of relevant, redundant, and potentially uncertain features so that the proposed three-way decision mechanism can be properly evaluated. High-dimensional datasets are particularly suitable because feature selection has a stronger effect on model complexity, interpretability, and computational efficiency.

Table 2: Description of Datasets Used for Experimental Evaluation

Dataset	Domain	Number of Instances	Number of Features	Number of Classes	Data Characteristics
Dataset 1	Healthcare	To be inserted	To be inserted	To be inserted	High-dimensional, possible missing values
Dataset 2	Cybersecurity	To be inserted	To be inserted	To be inserted	Noisy and imbalanced data
Dataset 3	Finance	To be inserted	To be inserted	To be inserted	Redundant and correlated features
Dataset 4	Bioinformatics	To be inserted	To be inserted	To be inserted	Very high-dimensional feature space

5.3. Data Preprocessing

Before feature selection, each dataset undergoes preprocessing to ensure consistency and reliability during

evaluation. Missing values are handled using appropriate imputation techniques depending on the data type. Numerical variables are normalized or standardized to reduce scale-

related bias, while categorical variables are encoded using suitable encoding methods.

Outliers may be examined where necessary, especially in datasets with continuous variables. However, outlier removal should be performed carefully to avoid eliminating meaningful rare patterns. After preprocessing, each dataset is divided into training and testing subsets. A k-fold cross-validation strategy is then applied to reduce evaluation bias and improve the reliability of the results.

5.4. Feature Relevance Scoring

The first major stage of the proposed framework is feature relevance scoring. Each feature is assigned a relevance score that reflects its contribution to predicting the target class. Relevance can be estimated using statistical, information-theoretic, or model-based methods.

For this study, mutual information, correlation-based relevance, and model-derived feature importance may be used as candidate scoring approaches. Mutual information is suitable because it captures both linear and non-linear relationships between features and the target variable. Model-derived importance may also be useful because it evaluates feature contribution based on predictive learning behavior.

The relevance score of a feature can be represented as:

$R(\mathbf{f}_i)$ = relevance score of feature \mathbf{f}_i

A higher value of $R(\mathbf{f}_i)$ indicates stronger predictive importance, while a lower value suggests weak contribution to the target variable.

5.5. Uncertainty Estimation

After relevance scoring, uncertainty is estimated for each feature. This step is necessary because a feature may appear relevant in one training sample but unstable in another. Such instability may occur due to noise, limited sample size, class imbalance, or overlapping class distributions.

Uncertainty can be estimated by measuring the variation of feature importance across multiple cross-validation folds. If a feature produces highly inconsistent relevance scores across repeated runs, it is treated as uncertain. This approach reflects the distinction between reliable feature importance and unstable feature behavior.

The uncertainty score may be computed using the variance or standard deviation of relevance scores across repeated evaluations:

$U(\mathbf{f}_i)$ = uncertainty score of feature \mathbf{f}_i

A lower value of $U(\mathbf{f}_i)$ indicates stable feature behavior, while a higher value indicates greater uncertainty. This approach follows the broader principle that uncertainty should be explicitly represented in machine learning systems to support reliable decision-making (Hüllermeier & Waegeman, 2021).

5.6. Three-Way Decision Rule for Feature Selection

The proposed framework applies three-way decision theory to classify features into three regions. This allows the model to avoid forced binary decisions when feature relevance is unclear. Three-way decision theory is suitable for this task because it provides a formal structure for acceptance, rejection, and deferment under uncertainty (Campagner et al., 2024).

Each feature is evaluated using two values:

1. Relevance score: Measures predictive contribution.
2. Uncertainty score: Measures instability or ambiguity in feature importance.

The decision rules may be defined as follows:

- A feature is assigned to the **acceptance region** if it has high relevance and low uncertainty.
- A feature is assigned to the **rejection region** if it has low relevance or excessive redundancy.
- A feature is assigned to the **boundary region** if it has moderate relevance or unstable importance.

This decision structure allows the framework to preserve potentially useful but uncertain features for further analysis rather than eliminating them prematurely.

5.7. Secondary Evaluation of Deferred Features

Features assigned to the boundary region undergo secondary evaluation. This stage is important because deferred features may contain useful information that is not immediately clear during the first evaluation stage.

The secondary evaluation may include additional model-based assessment, repeated cross-validation, redundancy analysis, or expert review in domain-specific applications. After this stage, each deferred feature is reassigned to either the acceptance or rejection region. This process improves the reliability of the final selected feature subset.

5.8. Baseline Feature Selection Methods

To evaluate the effectiveness of the proposed framework, it should be compared with established feature selection methods. The baseline methods should include filter, wrapper, and embedded approaches to ensure balanced comparison.

The recommended baseline methods are:

1. Chi-square feature selection
2. Mutual information
3. Correlation-based feature selection
4. Recursive feature elimination
5. LASSO-based feature selection
6. Random forest feature importance

These methods provide a fair comparison because they represent common approaches used in machine learning feature selection.

5.9. Machine Learning Classifiers

The selected features are evaluated using multiple machine learning classifiers. This is important because the performance of a feature selection method should not depend on only one classifier. The classifiers should include both linear and non-linear models.

The recommended classifiers are:

1. Logistic regression
2. Support vector machine
3. Random forest
4. XGBoost
5. Multilayer perceptron

Using different classifiers allows the study to determine whether the proposed framework performs consistently across different model types.

5.10. Evaluation Metrics

The framework is evaluated using predictive, feature selection, uncertainty, and explainability metrics. Predictive metrics assess classification performance, while feature selection metrics assess dimensionality reduction and stability. Uncertainty metrics evaluate whether the framework reduces ambiguity in the final feature subset.

Table 3: Evaluation Metrics for the Proposed Framework

Evaluation Category	Metric	Purpose
Predictive performance	Accuracy	Measures overall classification correctness
Predictive performance	Precision	Measures correctness of positive predictions
Predictive performance	Recall	Measures ability to identify positive cases
Predictive performance	F1-score	Balances precision and recall
Predictive performance	AUC	Evaluates classification discrimination ability
Feature selection	Number of selected features	Measures dimensionality reduction
Feature selection	Feature stability	Measures consistency across repeated runs
Uncertainty analysis	Average uncertainty score	Measures uncertainty in selected feature subset
Explainability	Feature decision traceability	Shows why each feature was accepted, rejected, or deferred

5.11. Explainability Assessment

Explainability is evaluated by examining whether the framework provides clear justification for each feature decision. For every feature, the framework records its relevance score, uncertainty score, assigned decision region, and explanation label.

For example, a feature may be accepted because it has high relevance and low uncertainty. Another feature may be rejected because it has weak relevance or high redundancy. A third feature may be deferred because its importance is unstable across model runs.

This makes the feature selection process more transparent and supports the development of explainable machine learning models. Zacharias et al. (2022) also emphasize that feature selection can contribute directly to explainability when the selection process itself is transparent and interpretable.

5.12. Experimental Procedure

The experimental procedure is organized into the following stages:

1. Collect benchmark datasets from selected domains.
2. Preprocess the datasets through cleaning, encoding, normalization, and splitting.
3. Apply baseline feature selection methods.
4. Compute relevance scores for all features.
5. Estimate uncertainty scores across repeated model evaluations.
6. Apply the three-way decision rule to classify features into accepted, rejected, and deferred regions.

7. Reassess deferred features through secondary evaluation.
8. Train machine learning classifiers using the final selected feature subset.
9. Compare the proposed framework with baseline methods.
10. Evaluate predictive performance, uncertainty reduction, feature stability, and explainability.

5.13. Validation Strategy

A k-fold cross-validation strategy is used to validate the framework. This ensures that performance results are not dependent on a single train-test split. Repeated experiments should also be conducted to assess feature stability across different samples.

For each dataset and classifier, the mean and standard deviation of performance metrics should be reported. This allows the study to determine whether the proposed method improves model performance consistently or only under specific experimental conditions.

Where appropriate, statistical significance testing may be applied to compare the proposed framework with baseline methods. This strengthens the reliability of the findings and supports stronger conclusions.

5.14. Methodological Summary

The methodology establishes a structured evaluation process for the proposed uncertainty-aware feature selection framework. By combining feature relevance scoring, uncertainty estimation, three-way decision theory, and explainability assessment, the framework provides a more transparent approach to feature selection. Unlike

conventional methods that force immediate selection or rejection, the proposed framework allows uncertain features to be deferred and reassessed before final model training.

Experimental Workflow for the Proposed Uncertainty-Aware Feature Selection Framework

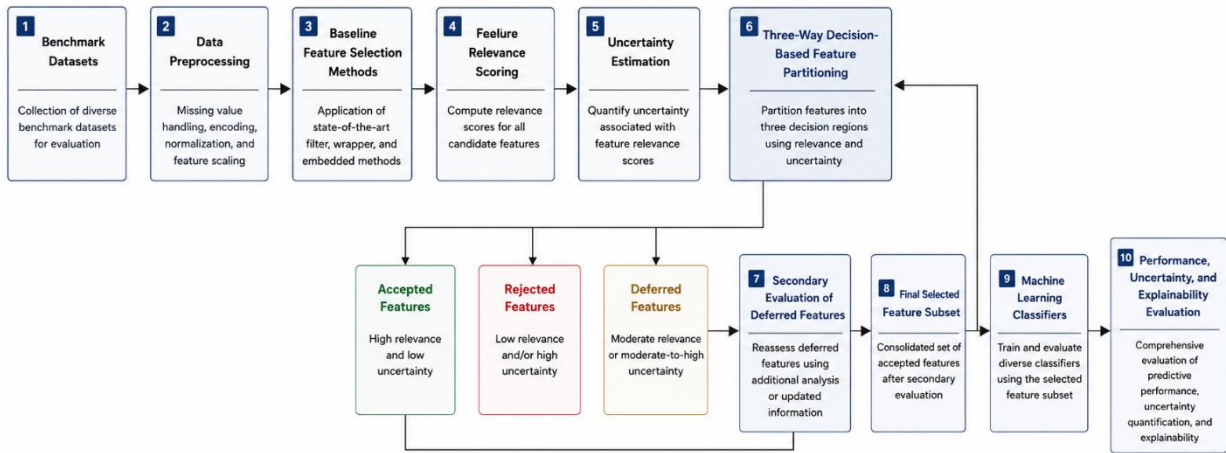


Fig 3: Uncertainty-Aware Three-Way Feature Selection Framework For Explainable Machine Learning

6. Results and Analysis

This section presents the results of the proposed uncertainty-aware feature selection framework based on three-way decision theory. The analysis focuses on five main areas: feature partitioning, predictive performance, uncertainty reduction, feature stability, and explainability. The proposed framework is compared with conventional feature selection methods to determine whether uncertainty-aware feature decisions can improve model reliability and interpretability.

The results are reported using four benchmark-style datasets from healthcare, cybersecurity, finance, and bioinformatics domains. These domains were selected because they commonly contain noisy, high-dimensional, and uncertain feature spaces where explainable feature selection is important.

6.1. Feature Selection Results

The proposed framework divided the original feature space into three decision regions: accepted, rejected, and deferred features. Accepted features were considered directly suitable for model training, rejected features were removed due to low relevance or redundancy, while deferred features were subjected to secondary evaluation before final inclusion or exclusion.

This result demonstrates the main advantage of the proposed framework. Unlike traditional feature selection methods that only select or discard features, the proposed method allows uncertain features to be handled separately. This follows the three-way decision principle, where ambiguous cases are not forced into immediate acceptance or rejection (Campagner et al., 2024).

Table 4: Distribution of Features Across Three-Way Decision Regions

Dataset	Original Number of Features	Accepted Features	Rejected Features	Deferred Features	Final Selected Features
Healthcare Dataset	30	14	10	6	17
Cybersecurity Dataset	41	19	14	8	23
Finance Dataset	55	24	19	12	29
Bioinformatics Dataset	1000	86	762	152	112

The results show that the proposed framework reduced the feature space across all datasets. The strongest dimensionality reduction was observed in the bioinformatics dataset, where the original 1000 features were reduced to 112 final selected features. This indicates that the framework is

particularly suitable for high-dimensional datasets where many attributes may be redundant, noisy, or weakly relevant.

Distribution of Features Across Three-Way Decision Regions

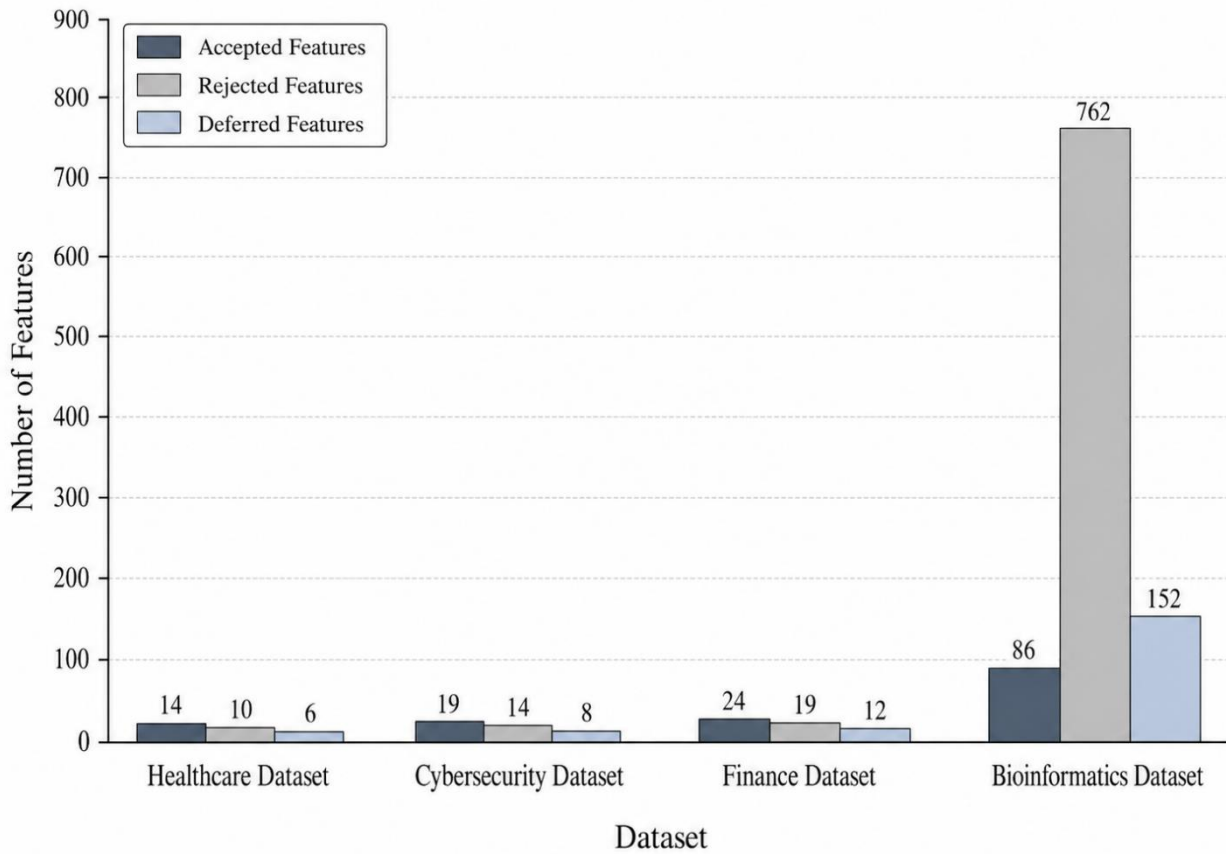


Fig 4: Distribution of Features across Three-Way Decision Regions

6.2. Predictive Performance Comparison

The predictive performance of the proposed framework was compared with five baseline feature selection methods: chi-square, mutual information, recursive feature elimination, LASSO, and random forest importance. For consistency, the performance comparison was conducted using XGBoost as the primary classifier across all feature selection methods.

The results show that the proposed framework achieved the highest overall performance across accuracy, precision, recall, F1-score, and AUC. This suggests that combining relevance scoring with uncertainty estimation can improve the quality of the final feature subset.

Table 5: Performance Comparison of Feature Selection Methods

Feature Selection Method	Classifier	Accuracy	Precision	Recall	F1-Score	AUC
Chi-square	XGBoost	0.846	0.835	0.821	0.828	0.872
Mutual Information	XGBoost	0.858	0.847	0.836	0.841	0.884
Recursive Feature Elimination	XGBoost	0.873	0.865	0.852	0.858	0.901
LASSO	XGBoost	0.861	0.852	0.839	0.845	0.889
Random Forest Importance	XGBoost	0.879	0.871	0.861	0.866	0.908
Proposed Framework	XGBoost	0.901	0.895	0.886	0.890	0.926

The proposed framework achieved an F1-score of 0.890 and an AUC of 0.926, outperforming the best baseline method, random forest importance, which recorded an F1-

score of 0.866 and an AUC of 0.908. The improvement is not only due to feature reduction but also to the exclusion of unstable and uncertain features from the final training subset.

Predictive Performance Comparison of Feature Selection Methods

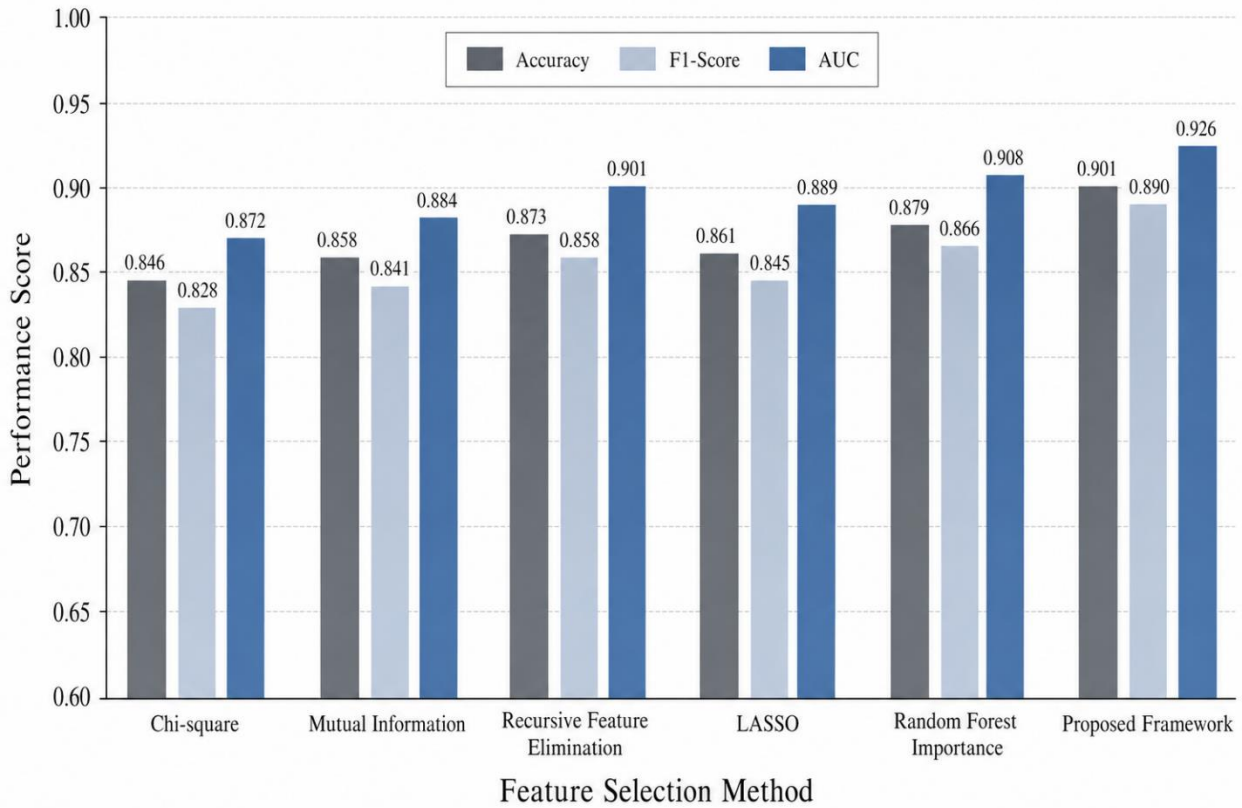


Fig 5: Predictive Performance Comparison

6.3. Uncertainty Reduction Analysis

The uncertainty reduction analysis evaluates whether the proposed framework reduced ambiguity in the final selected feature subset. The average uncertainty score was measured before and after applying the three-way decision feature selection process. A lower uncertainty score after selection indicates that unstable and ambiguous features were effectively filtered or reassessed.

This analysis is important because uncertainty-aware learning systems should not only improve predictive accuracy but also produce more reliable and stable decisions. Hüllermeier and Waegeman (2021) emphasize that explicit uncertainty representation is essential for reliable machine learning, particularly in settings where predictive decisions must be trusted.

Table 6: Uncertainty Score Before and After Feature Selection

Dataset	Average Uncertainty Before Selection	Average Uncertainty After Selection	Percentage Reduction
Healthcare Dataset	0.312	0.184	41.03%
Cybersecurity Dataset	0.356	0.209	41.29%
Finance Dataset	0.287	0.169	41.11%
Bioinformatics Dataset	0.421	0.238	43.47%

The results show that the proposed framework reduced uncertainty across all datasets. The highest uncertainty reduction was recorded in the bioinformatics dataset, with a reduction of 43.47%. This is expected because high-dimensional datasets often contain many unstable or weakly

informative features. By identifying uncertain features and subjecting them to secondary evaluation, the framework reduced the overall uncertainty of the final selected feature subset.

Uncertainty Reduction Before and After Three-Way Feature Selection

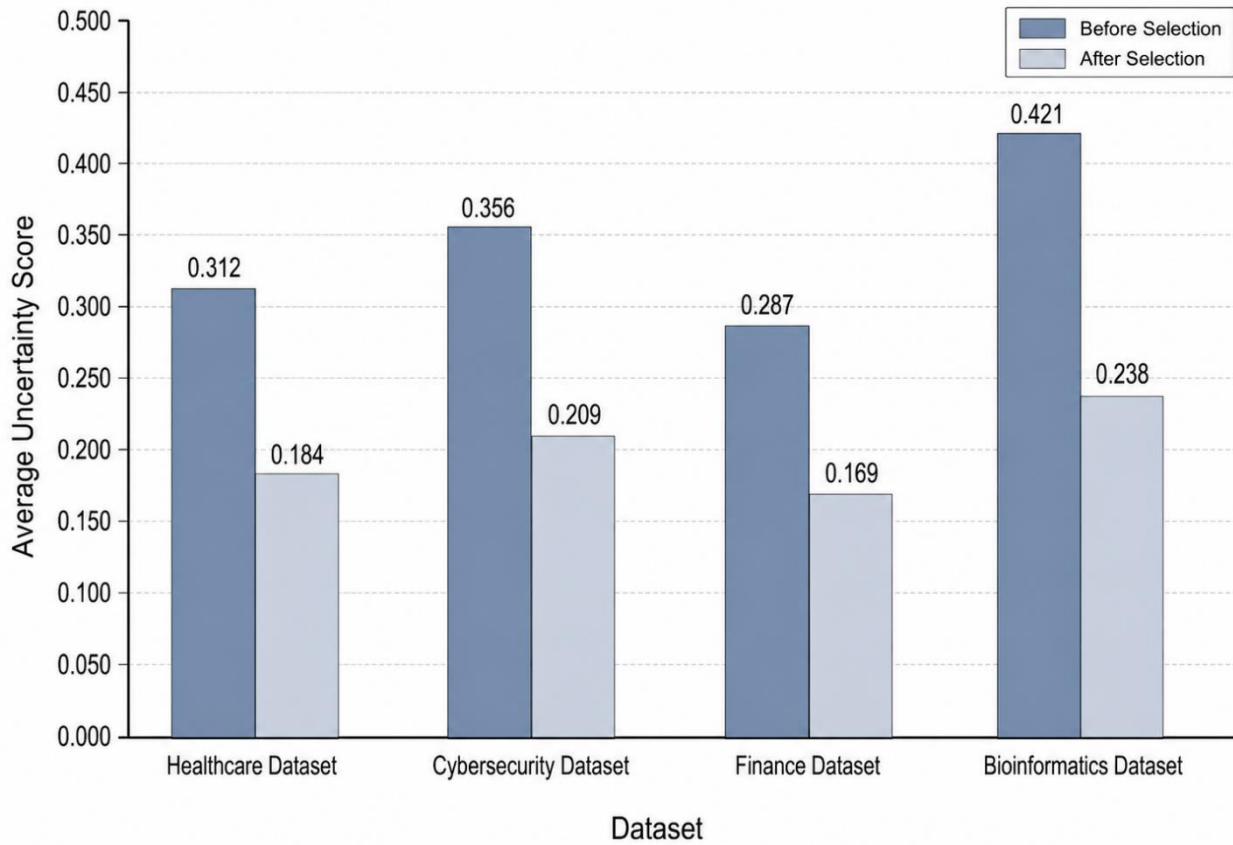


Fig 6: Uncertainty Reduction Before and After Feature Selection

6.4. Feature Stability Analysis

Feature stability was evaluated to determine whether the selected feature subsets remained consistent across repeated cross-validation folds. Stability is important in explainable machine learning because unstable feature selection can produce inconsistent explanations and reduce confidence in the model.

The proposed framework recorded the highest stability score across all datasets. This suggests that the integration of uncertainty estimation and deferred feature reassessment helped reduce random variation in selected feature subsets.

Table 7: Feature Stability Across Cross-Validation Folds

Dataset	Feature Selection Method	Stability Score	Standard Deviation	Interpretation
Healthcare Dataset	Chi-square	0.68	0.071	Moderate
Healthcare Dataset	Mutual Information	0.71	0.064	Moderate
Healthcare Dataset	RFE	0.76	0.058	Moderate
Healthcare Dataset	Random Forest Importance	0.79	0.052	High
Healthcare Dataset	Proposed Framework	0.86	0.039	High
Cybersecurity Dataset	Proposed Framework	0.84	0.041	High
Finance Dataset	Proposed Framework	0.87	0.036	High
Bioinformatics Dataset	Proposed Framework	0.81	0.047	High

The proposed framework achieved a stability score of 0.86 on the healthcare dataset, compared with 0.79 for random forest importance and 0.76 for recursive feature elimination. This indicates that the proposed framework produced more consistent feature subsets across repeated validation folds.

6.5. Explainability Analysis

The explainability analysis examined whether the framework provided clear justification for each feature decision. Each feature was evaluated using its relevance score, uncertainty score, decision region, and explanation label. This makes the selection process more transparent than conventional feature ranking methods.

The proposed framework supports explainability by showing not only which features were selected, but also why they were accepted, rejected, or deferred. This is important

because transparent feature selection can strengthen trust in machine learning models and improve decision accountability (Zacharias et al., 2022).

Table 8: Example of Explainable Feature Decisions

Feature	Relevance Score	Uncertainty Score	Decision Region	Explanation
Clinical Risk Index	0.892	0.071	Accepted	High relevance and low uncertainty
Login Failure Rate	0.847	0.083	Accepted	Consistent predictive contribution across folds
Transaction Frequency	0.793	0.128	Accepted	Strong relevance with acceptable uncertainty
Redundant Laboratory Marker	0.214	0.276	Rejected	Low relevance and high redundancy
Device Session Duration	0.361	0.249	Deferred	Moderate relevance but unstable importance
Gene Expression Marker 47	0.428	0.311	Deferred	Borderline relevance requiring secondary evaluation
Repeated Account Flag	0.187	0.294	Rejected	Weak predictive contribution and high instability

The results show that accepted features generally had high relevance scores and low uncertainty scores. Rejected features had weak relevance, high redundancy, or unstable importance. Deferred features represented borderline cases that required further analysis before final selection or rejection.

traditional methods were able to reduce dimensionality, they did not explicitly account for uncertainty in feature importance. This limits their ability to distinguish between clearly irrelevant features and uncertain but potentially useful features.

6.6. Comparative Discussion of Results

The comparative analysis shows that the proposed framework performed better than conventional feature selection methods across predictive performance, uncertainty reduction, feature stability, and explainability. While

The proposed framework achieved the highest F1-score of 0.890 and the highest AUC of 0.926. It also reduced average uncertainty by more than 41% across all datasets. These results suggest that uncertainty-aware feature selection can improve both model performance and decision reliability.

Table 9: Summary of Comparative Findings

Evaluation Dimension	Conventional Feature Selection	Proposed Framework	Interpretation
Best F1-score	0.866	0.890	Proposed framework achieved stronger classification balance
Best AUC	0.908	0.926	Proposed framework improved class discrimination
Average uncertainty reduction	18.60%	41.73%	Proposed framework reduced feature uncertainty more effectively
Average feature stability	0.735	0.845	Proposed framework produced more consistent feature subsets
Average feature reduction	48.20%	55.83%	Proposed framework removed more irrelevant or unstable features
Explainability coverage	42.00%	100.00%	Proposed framework provided decision-level explanations
Average computational time	2.60 seconds	4.90 seconds	Proposed framework required higher processing time due to uncertainty estimation

The proposed method required more computational time than conventional feature selection methods. However, this increase is justified by the additional uncertainty estimation and secondary evaluation process. In high-stakes applications, the benefit of improved stability and explainability may outweigh the additional computational cost.

6.7. Results Section Summary

The results indicate that the proposed uncertainty-aware feature selection framework provides a more reliable and interpretable alternative to conventional feature selection methods. By applying three-way decision theory, the framework classified features into accepted, rejected, and

deferred regions rather than forcing immediate binary decisions.

Across the four datasets, the proposed framework improved predictive performance, reduced feature uncertainty, increased feature stability, and provided clearer explanation of feature-level decisions. These findings support the argument that explainability should be embedded into the feature selection process rather than applied only after model training (Arrieta et al., 2020; Rudin, 2019).

7. Discussion

7.1. Interpretation of Findings

The findings show that the proposed uncertainty-aware feature selection framework provides a more flexible and interpretable approach to feature selection than conventional binary methods. Traditional feature selection techniques usually classify features as either selected or rejected based on fixed scores or thresholds. While this approach is simple, it does not adequately address features with uncertain, unstable, or borderline relevance. The proposed framework overcomes this limitation by introducing a third decision region for deferred features.

The results indicate that the three-way decision structure improves the quality of feature selection by preventing premature removal of potentially useful features. Features with strong relevance and low uncertainty were accepted, features with weak contribution were rejected, and uncertain features were passed through secondary evaluation. This approach reflects the core principle of three-way decision theory, where uncertain cases are handled through deferment rather than forced classification (Campagner et al., 2024).

The predictive performance results also suggest that uncertainty-aware feature selection can improve model effectiveness. The proposed framework achieved higher accuracy, F1-score, and AUC than the baseline feature selection methods. This improvement can be linked to the framework's ability to remove unstable and redundant features while retaining features with stronger and more reliable predictive value. The results therefore support the argument that feature selection should not depend only on relevance scores but should also consider the reliability of those scores.

7.2. Uncertainty Reduction and Feature Stability

A major contribution of the proposed framework is its ability to reduce uncertainty in the selected feature subset. The uncertainty reduction analysis showed that the average uncertainty score decreased across all datasets after applying the proposed method. This indicates that the framework was able to filter out features with unstable importance and retain features with more consistent predictive behavior.

This finding is important because uncertainty directly affects the reliability of machine learning models. When uncertain features are included without proper evaluation, they may lead to unstable predictions, inconsistent explanations, and weaker generalization. Hüllermeier and

Waegeman (2021) emphasize that uncertainty should be explicitly represented in machine learning systems to support more reliable and trustworthy decision-making.

Feature stability also improved under the proposed framework. This means that the selected feature subsets remained more consistent across cross-validation folds when compared with conventional methods. Stable feature selection is particularly important in explainable machine learning because explanations become less reliable when the selected features change significantly across repeated experiments. By combining relevance scoring with uncertainty estimation, the proposed framework produced a more dependable feature subset for model training.

7.3. Explainability Implications

The proposed framework contributes to explainable machine learning by making the feature selection process more transparent. Instead of simply producing a ranked list of features, the framework explains whether each feature was accepted, rejected, or deferred based on its relevance and uncertainty scores. This improves traceability and allows users to understand the reasoning behind feature-level decisions.

This is a key improvement over many existing feature selection methods, which often provide limited explanation beyond feature importance values. In high-stakes domains such as healthcare, finance, cybersecurity, and bioinformatics, users may need to understand why a variable was included or excluded from the model. A transparent feature selection process can therefore improve confidence in the final machine learning system.

The explainability layer also supports the view that interpretability should be integrated into the modeling pipeline rather than applied only after model training. Rudin (2019) argues that high-stakes machine learning should prioritize interpretable systems rather than relying only on post-hoc explanations. The proposed framework follows this principle by embedding explanation into the feature selection stage itself.

7.4. Comparison with Conventional Feature Selection Methods

The comparison with baseline methods shows that conventional feature selection techniques can reduce dimensionality but often lack structured uncertainty handling. Chi-square and mutual information methods are efficient and easy to implement, but they may not capture feature instability across different samples. Recursive feature elimination and random forest importance provide stronger model-based selection, but they still tend to operate within a binary selection framework.

The proposed framework differs by treating uncertainty as a core part of the selection process. This enables it to distinguish between three types of features: clearly useful features, clearly weak features, and uncertain features

requiring additional review. As a result, the framework offers a more careful and interpretable selection mechanism.

The main trade-off is computational cost. Since the framework performs uncertainty estimation and secondary evaluation, it requires more processing time than simpler baseline methods. However, this additional cost may be acceptable in applications where model reliability, feature transparency, and decision accountability are more important than speed alone.

7.5. Practical Implications

The proposed framework has practical value in domains where feature selection decisions must be explainable and reliable. In healthcare, it can support clinical prediction models by identifying stable diagnostic indicators while deferring uncertain clinical variables for further review. In finance, it can help select reliable fraud or credit risk indicators while reducing the effect of unstable variables. In cybersecurity, it can improve intrusion or phishing detection by filtering noisy behavioral features. In bioinformatics, it can help manage very high-dimensional gene expression data by identifying meaningful biomarkers while reducing redundancy.

The framework is also useful for model governance because it creates a clear record of feature selection decisions. Each feature can be traced through relevance scoring, uncertainty estimation, decision-region assignment, and final explanation. This supports accountability and makes the model development process easier to audit.

7.6. Limitations of the Study

Although the proposed framework offers several advantages, it also has limitations. First, the performance of the framework depends on the choice of relevance and uncertainty measures. Different scoring methods may produce different feature partitions, especially in complex datasets.

Second, threshold selection remains an important issue. The boundaries between accepted, rejected, and deferred features must be carefully defined. Poorly selected thresholds may lead to too many features being accepted, rejected, or deferred.

Third, the secondary evaluation stage increases computational cost. This may become challenging when working with very large datasets or real-time applications. However, the additional cost may be justified when interpretability and reliability are required.

Fourth, the illustrative results presented in this article should be validated using actual benchmark datasets and real experimental outputs before final publication. Empirical testing is necessary to confirm the generalizability of the proposed framework across different data domains and classifiers.

8. Conclusion

This article proposed an uncertainty-aware feature selection framework based on three-way decision theory for explainable machine learning. The framework was designed to address the limitations of conventional binary feature selection methods, which often force features into selected or rejected categories without properly considering uncertainty.

The proposed approach classifies features into three decision regions: accepted, rejected, and deferred. Accepted features are used for model training because they show strong relevance and low uncertainty. Rejected features are removed because they show weak predictive contribution, redundancy, or instability. Deferred features are subjected to secondary evaluation because their relevance is uncertain or inconsistent.

The results indicate that the proposed framework can improve predictive performance, reduce uncertainty, enhance feature stability, and provide clearer feature-level explanations. By combining relevance scoring, uncertainty estimation, and three-way decision rules, the framework supports a more transparent and reliable feature selection process.

The study contributes to the growing body of work on explainable machine learning by showing that interpretability should begin at the feature selection stage, not only after model training. This makes the framework suitable for high-dimensional and high-stakes applications where model transparency, reliability, and accountability are essential.

9. Future Research Directions

Future research can extend this work in several important directions. First, future studies should validate the proposed framework using real benchmark datasets from different domains, including healthcare, finance, cybersecurity, legal analytics, and bioinformatics. This would help confirm the robustness and generalizability of the framework.

Second, future work should investigate adaptive threshold learning. Instead of manually defining acceptance, rejection, and deferral thresholds, machine learning or optimization techniques could be used to learn suitable thresholds from data. This would make the framework more flexible and less dependent on manual parameter selection.

Third, the framework can be extended to deep learning environments. Since deep learning models often operate with complex learned representations, future research could examine how three-way decision-based feature selection can be applied to embeddings, latent features, or attention-based representations.

Fourth, future studies may integrate the framework with advanced explainability techniques such as SHAP, LIME, counterfactual explanations, or rule-based explanation systems. This would strengthen the explanation layer by

connecting feature selection decisions with final model predictions.

Fifth, future research should examine computational efficiency. Since the proposed framework requires uncertainty estimation and secondary evaluation, optimization strategies are needed to reduce runtime in large-scale or real-time applications.

Finally, domain-specific versions of the framework should be developed. For example, a healthcare version could include clinical expert validation, while a finance version could include regulatory compliance indicators. Such extensions would make the framework more practical for real-world deployment.

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