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Monotonicity Constraints in Multiclass XGBoost: One-vs-Rest Concept and Class-Specific Constraints

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Abstract: Machine learning interpretability has emerged as a critical requirement in high-stakes applications where transparent decision-making processes are essential for regulatory compliance and expert validation. This article presents a novel framework for implementing monotonicity constraints in multiclass XGBoost systems through the one-vs-rest decomposition strategy, addressing the fundamental challenge of maintaining interpretable feature-prediction relationships across multiple class outputs simultaneously. The proposed framework introduces a constraint matrix representation that enables class-specific monotonicity specifications while ensuring global consistency through sophisticated coordination algorithms. The implementation modifies the traditional XGBoost tree-building process to incorporate per-class constraint-aware splitting criteria that balance predictive accuracy with interpretability requirements. Advanced loss function modifications augment standard multiclass cross-entropy with adaptive penalty terms that quantify constraint violations across all classes. This is a modification of the current XGBoost multi-class implementation, where only one constraint relationship can be defined for all the classes, limiting accurate business-aligned interpretability. Benchmarking results demonstrate that the framework successfully maintains interpretability without significant accuracy degradation, particularly excelling in domains with inherent monotonic relationships such as credit scoring and medical diagnosis. The constraint enforcement during training provides stronger guarantees about model behavior compared to post-hoc interpretability methods, ensuring that monotonic relationships are preserved throughout the model lifecycle rather than approximated after training completion.

Keywords: Monotonicity constraints, multiclass classification, XGBoost, interpretable machine learning, constraint-based optimization, Explanability in AI.

INTRODUCTION

Machine learning interpretability has become increasingly critical in high-stakes applications where understanding feature-prediction relationships is as important as achieving high accuracy. The fundamental challenge of explaining model predictions has driven significant research into constraint-based approaches that ensure model behavior aligns with domain knowledge and expectations (Ribeiro, M. T. *et al.*, 2016). Monotonicity constraints in gradient boosting frameworks like XGBoost offer a powerful mechanism to ensure that predictions follow expected directional relationships with input features. These constraints address the growing demand for transparent and accountable AI systems in sectors where regulatory compliance and expert validation are mandatory requirements. While these constraints have been successfully implemented in regression and binary classification scenarios, their extension to multiclass problems presents both theoretical and practical challenges that require sophisticated algorithmic innovations (Molnar, C. 2020). The multiclass classification paradigm, particularly when implemented through the one-vs-rest approach, creates multiple binary decision boundaries simultaneously, each requiring independent constraint evaluation and coordination mechanisms to maintain global consistency across all class predictions.

The emergence of explainable artificial intelligence has fundamentally shifted the research focus from purely performance-driven models to interpretable systems that can provide meaningful insights into their decision-making processes. This paradigm shift has been particularly pronounced in domains such as healthcare, finance, and criminal justice, where algorithmic decisions can have profound impacts on human lives and societal outcomes. The development of monotonicity constraints represents a significant advancement in this direction, providing a principled approach to incorporating domain expertise directly into the learning process while maintaining the predictive power of modern machine learning algorithms. Furthermore, the increasing regulatory scrutiny of automated decision-making systems has created an urgent need for methods that can demonstrate compliance with fairness and transparency requirements, making constraint-based approaches not just desirable but often legally necessary.

BACKGROUND AND THEORETICAL FOUNDATION

Traditional monotonicity constraints in XGBoost operate under the assumption of a single target variable with clear directional relationships to input features, building upon the fundamental principles of scalable tree boosting systems that have revolutionized machine learning applications across diverse domains (Chen, T., & Guestrin, C.

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2016). In regression tasks, a monotonic constraint ensures that increasing values of a specified feature lead to non-decreasing predictions, maintaining mathematical consistency throughout the prediction surface. Binary classification extends this concept by applying constraints to the logit transformation of class probabilities, ensuring that the underlying decision boundaries respect the specified monotonic relationships while preserving the probabilistic interpretation of the outputs. The XGBoost framework provides built-in support for monotonic constraints in these simpler scenarios, demonstrating the practical feasibility and computational efficiency of constraint-based learning approaches (XGBoost).

When building trees, XGBoost evaluates splits using the **similarity score** and **gain** equations. Under monotonicity constraints, it **filters out** splits that violate the specified directionality (Chen, T., & Guestrin, C. 2016).

$$Similarity\ Score(SS) = (\sum_i g_i)^2/(\sum_i h_i + \lambda)$$

$$Gain = \mathrm{G_L}^2/(H_L + \lambda) + \mathrm{G_R}^2/(H_R + \lambda) - \mathrm{G}^2/(H + \lambda) - \gamma$$

When a feature *f* is constrained, the relative position of the left and right child nodes must adhere to the expected prediction ordering:

For +1: $w_R \geq w_L$

For −1: $w_R \leq w_L$

Where leaf weights are computed as:

$$w_j = -\sum_{i \in j} g_i /(\sum_{i \in j} h_i + \lambda)$$

The mathematical foundation of monotonicity constraints relies on restricting the splitting criteria during tree construction (refer to the above formulations), fundamentally altering the tree-building process to incorporate domain knowledge alongside data-driven optimization objectives. For a feature with a monotonic increasing constraint, all splits must satisfy the condition that leaf values in the right subtree are greater than or equal to those in the left subtree, creating a hierarchical constraint propagation mechanism that ensures consistency across all tree levels. This constraint propagation mechanism becomes significantly more complex in multiclass scenarios where multiple output classes compete for optimal feature splits, requiring sophisticated coordination algorithms to prevent constraint violations while maintaining predictive accuracy. The theoretical framework must account for the interaction between different constraint types and their cumulative effect on model capacity and generalization performance.

The one-vs-rest decomposition strategy transforms a k-class problem into k binary classification problems, where each binary classifier distinguishes one class from all remaining classes, creating opportunities for class-specific constraint specifications while introducing coordination challenges across the ensemble of binary classifiers. This decomposition creates opportunities for class-specific monotonicity constraints but also introduces coordination challenges across the ensemble of binary classifiers, requiring novel algorithmic approaches to ensure global consistency in the final multiclass prediction. The theoretical framework must address how constraints interact across different binary problems and ensure consistency in the final multiclass prediction, incorporating principles from ensemble learning theory and constrained optimization to maintain both interpretability and predictive performance.

The complexity of multiclass constraint enforcement extends beyond simple aggregation of binary classifiers, requiring sophisticated mathematical frameworks that can handle conflicting constraints and ensure global optimality. The theoretical foundation must account for scenarios where a feature might have different monotonic relationships with different classes, potentially creating contradictory requirements that need to be resolved through principled optimization strategies. Additionally, the framework must consider the impact of class imbalance on constraint satisfaction, as dominant classes might overshadow the constraint requirements of minority classes, leading to biased interpretations and suboptimal performance in real-world scenarios where balanced constraint satisfaction across all classes is crucial for fair and reliable decision-making.

Table 1: Constraint Mechanisms Comparison (Chen, T., & Guestrin, C. 2016; XGBoost)

Classification Type	Constraint Scope	Complexity Level	Coordination Requirements	Theoretical Foundation
Binary Classification	Single Decision Boundary	Low	Minimal	Well-Established
Regression	Continuous Output	Low	None	Mature Theory

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Multiclass (One-vs-All)	Multiple Boundaries	High	Extensive	Emerging Framework
Multiclass (One-vs-One)	Pairwise Boundaries	Very High	Complex	Limited Theory
Hierarchical Multiclass	Nested Boundaries	Medium	Moderate	Specialized Methods

PROPOSED METHODOLOGY AND PER-CLASS CONSTRAINT IMPLEMENTATION

Implementing per-class monotonicity constraints requires fundamental modifications to the XGBoost tree-building algorithm, drawing upon principles of large-scale machine learning with stochastic gradient descent to ensure computational efficiency in high-dimensional settings (Bottou, L. 2010). The proposed methodology introduces a constraint matrix C ∈ R^(k×p), where k represents the number of classes and p denotes the feature dimensionality, allowing for flexible specification of asymmetric constraint patterns that reflect the complex relationships between features and different class outcomes. Each element C[i,j] specifies the monotonicity constraint for feature j with respect to class i, enabling domain experts to encode their knowledge about feature-class relationships while maintaining algorithmic flexibility for automatic constraint discovery. This matrix-based representation facilitates efficient constraint evaluation and enables parallel processing across different classes and features.

We maintain K class-wise scorers $f_k(x)$, each trained as a constrained binary learner against "rest," but we compute a joint softmax cross-entropy at every boosting round to couple the updates across classes. At iteration(t), logits are $z_{ik}^{(t-1)} = f_k^{(t-1)}(x_i)$, probabilities come from the softmax $p_{ik} = \frac{e^{z_{ik}}}{\sum_{c=1}^{K} e^{z_{ic}}}$, and the loss is $L = -\sum_i \sum_{k=1}^{K} y_{ik} log p_{ik}$.

Using second-order optimization, gradients and (diagonal) Hessians with respect to each class-logit are $g_{ik} = p_{ik} - y_{ik}$ and $h_{ik} = p_{ik}(1-p_{ik})$. For each class (k), XGBoost fits a tree whose leaves j carry weights $w_{j,k} = -G_{j,k}/(H_{j,k}+\lambda)$ with $G_{j,k} = \sum_{i\in j} g_{ik}$ and $H_{j,k} = \sum_{i\in j} h_{ik}$, maximizing the split gain $G_{split,k} = \frac{G_{L,k}^2}{H_{L,k}+\lambda} + \frac{G_{R,k}^2}{H_{R,k}+\lambda} - \frac{G_{N,k}^2}{H_{N,k}+\lambda} - \gamma$. Class-specific monotonicity constraints are encoded as signs $s_{m,k} \in \{-1,0,1\}$ per feature m and enforced on every candidate split of the class-k tree by requiring ordered leaf predictions along the split feature: if $s_{m,k} = +1$ then $\omega_{R,k} \geq \omega_{L,k}$, if $s_{m,k} = -1$ then $\omega_{R,k} \leq \omega_{L,k}$; violating splits are discarded.

The class-wise scorers are then updated additively with learning rate (η): $f_k^{(t)}(x) = f_k^{(t-1)}(x) + \eta h_k^{(t)}(x)$, and the coupled softmax is recomputed before the next round. Note: monotonicity is guaranteed for the class-k logit $f_k(x)$; to induce monotonicity in the probability $p_k(x)$, constraints across all classes should be aligned on that feature.

- Softmax and loss: $p_{ik} = \frac{e^{z_{ik}}}{\sum_{c=1}^{K} e^{z_{ic}}}$, $L = -\sum_i \sum_{k=1}^{K} y_{ik} log p_{ik}$
- Gradients/Hessians (per class logit): $g_{ik} = p_{ik} - y_{ik}$, $h_{ik} = p_{ik}(1-p_{ik})$
- Leaf weight and split gain for class k: $\omega_{j,k} = -\frac{\sum_{i\in j} g_{ik}}{\sum_{i\in j} h_{ik}+\lambda}$, $G_{split,k} = \frac{G_{L,k}^2}{H_{L,k}+\lambda} + \frac{G_{R,k}^2}{H_{R,k}+\lambda} - \frac{G_{N,k}^2}{H_{N,k}+\lambda} - \gamma$
- Monotonicity check on feature m for class k: $s_{m,k} = +1 \Rightarrow \omega_{R,k} \geq \omega_{L,k}$, $s_{m,k} = 11 \Rightarrow \omega_{R,k} \leq \omega_{L,k}$
- Additive update: $f_k^{(t)}(x) = f_k^{(t-1)}(x) + \eta h_k^{(t)}(x)$

The tree splitting procedure must be modified to evaluate constraint satisfaction for each class independently, incorporating decision-theoretic principles that balance immediate splitting gains with long-term constraint adherence (Freund, Y., & Schapire, R. E. 1997). During node splitting, the algorithm evaluates potential splits not only for their contribution to loss reduction but also for their compliance with class-specific monotonicity requirements, creating a multi-objective optimization problem that requires careful balancing of competing objectives. This dual optimization creates a constrained optimization problem that can be solved using Lagrangian methods or penalty-based approaches, incorporating techniques from convex optimization theory to ensure convergence to feasible solutions. The modified splitting criteria must account for the cumulative effect of constraint violations across all classes while maintaining computational efficiency suitable for large-scale applications.

Feature interaction effects pose additional complexity in the multiclass setting, requiring

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sophisticated analysis techniques that can handle high-dimensional feature spaces and complex interaction patterns. When features interact through multiplicative or other non-linear relationships, monotonicity constraints must be evaluated across the entire feature space rather than univariately, necessitating the development of interaction-aware constraint checking mechanisms. The methodology incorporates interaction-aware constraint checking that examines partial derivatives of the prediction function with respect to constrained features, ensuring monotonicity preservation even in the presence of complex feature dependencies that might otherwise lead to constraint violations in regions of the feature space not adequately represented in the training data.

The implementation strategy also addresses the challenge of constraint inheritance across tree levels, ensuring that constraints imposed at higher levels of the tree hierarchy are properly propagated to leaf nodes without creating contradictions or infeasible solutions. This requires the development of constraint validation algorithms that can efficiently verify the consistency of constraint specifications across the entire tree ensemble, detecting potential conflicts before they affect model performance. Additionally, the methodology incorporates adaptive constraint relaxation mechanisms that can temporarily loosen constraint requirements in regions of the feature space where strict adherence would result in significant performance degradation, while maintaining overall interpretability through selective constraint enforcement based on local data density and prediction confidence levels.

LOSS FUNCTION MODIFICATIONS AND OPTIMIZATION STRATEGIES

Novel loss functions specifically designed for constrained multiclass problems are essential for maintaining both accuracy and interpretability, building upon the theoretical foundations of greedy function approximation and gradient boosting methodologies (Friedman, J. H. 2001). The standard multiclass cross-entropy loss must be augmented with penalty terms that quantify constraint violations across all classes simultaneously, creating a unified objective function that balances predictive accuracy with constraint adherence. The modified loss function incorporates adaptive penalty weights that adjust dynamically based on the severity and frequency of constraint violations, ensuring that the optimization process converges to solutions that satisfy both accuracy and interpretability requirements. This approach requires careful tuning of penalty parameters to avoid over-penalization that might degrade predictive performance while ensuring sufficient constraint enforcement.

The penalty function design requires careful consideration of differentiability and computational efficiency to maintain gradient-based optimization compatibility, incorporating principles from the theory of weak learning and boosting algorithms (Schapire, R. E. 1990). Tree-splitting techniques must be redesigned to accommodate these modified loss functions, extending the standard greedy splitting approach with constraint-aware evaluation metrics that incorporate both immediate gain and long-term constraint satisfaction. The constraint-aware splitting criteria evaluate multiple potential splits simultaneously, considering their impact on both local node purity and global constraint satisfaction across all classes. This requires developing heuristics for evaluating potential constraint violations in future tree levels, creating a form of lookahead optimization that balances immediate performance gains with constraint compliance.

The optimization framework incorporates advanced regularization techniques that prevent overfitting while maintaining constraint satisfaction, utilizing cross-validation strategies to select optimal penalty parameters and constraint configurations. The modified optimization procedure must account for the increased complexity of the constraint-aware objective function while maintaining convergence guarantees and computational efficiency suitable for large-scale applications. Early stopping mechanisms are integrated to prevent excessive constraint enforcement that might lead to underfitting, while adaptive learning rate schedules ensure stable convergence in the presence of complex constraint interactions.

The development of robust optimization strategies requires careful consideration of the trade-offs between constraint satisfaction and model flexibility, particularly in scenarios where training data may not fully represent the feature space regions where constraints are most critical. The framework incorporates uncertainty quantification methods that can assess the reliability of constraint enforcement in different regions of the feature space, providing practitioners with insights into the confidence levels associated with monotonic relationships in their trained models. Furthermore, the optimization strategy includes mechanisms for

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handling noisy or contradictory training data that might appear to violate expected monotonic relationships, utilizing robust statistical methods to distinguish between genuine constraint violations and data quality issues that should not influence the constraint enforcement process.

Table 2: Penalty Function Comparison (Friedman, J. H. 2001; Schapire, R. E. 1990)

Penalty Function	Differentiability	Computational Cost	Convergence Rate	Constraint Violation Handling
Quadratic Penalty	Smooth	Low	Fast	Soft Violation
Absolute Penalty	Non-smooth	Medium	Moderate	Hard Violation
Logarithmic Barrier	Smooth	High	Slow	Barrier Method
Adaptive Hybrid	Smooth	Medium	Fast	Dynamic Adjustment
Exponential Penalty	Smooth	Medium	Variable	Severity-Based

COMPUTATIONAL EFFICIENCY AND SCALABILITY CONSIDERATIONS

Large-scale distributed computing environments present unique challenges for implementing per-class monotonicity constraints, requiring sophisticated approaches to parallel processing and distributed optimization that build upon established frameworks for cluster computing (Zaharia, M. *et al.*, 2010). The constraint evaluation process introduces additional computational overhead that scales with both the number of classes and features, necessitating the development of efficient algorithms that minimize this overhead while maintaining constraint integrity across distributed workers. Parallel constraint evaluation strategies leverage the independence of class-specific constraints to distribute computation across multiple processing units, utilizing load-balancing techniques to ensure optimal resource utilization across the computing cluster. Each worker can evaluate constraints for a subset of classes, with coordination required only during the final aggregation step, minimizing communication overhead while maintaining scalability for high-dimensional multiclass problems.

The distributed implementation must address challenges related to data partitioning, constraint synchronization, and fault tolerance, incorporating principles from MapReduce and similar distributed computing paradigms (Dean, J., & Ghemawat, S. 2008). Memory optimization techniques are crucial for handling large constraint matrices in distributed environments, utilizing sparse representation strategies that exploit the common scenario where only a subset of features requires monotonicity constraints for each class. Compressed storage formats and lazy evaluation mechanisms further reduce memory footprint while maintaining computational efficiency, enabling the processing of datasets with millions of samples and thousands of features across distributed computing clusters.

The scalability analysis must consider both computational and memory requirements as the problem size increases, incorporating theoretical complexity analysis and empirical performance evaluation across different cluster configurations. Advanced caching strategies and data locality optimizations ensure efficient memory access patterns that minimize network communication and maximize computational throughput. The distributed architecture incorporates fault tolerance mechanisms that maintain constraint consistency even in the presence of node failures or network partitions, ensuring robust operation in production environments where system reliability is critical.

The implementation of distributed constraint evaluation requires sophisticated coordination protocols that can handle dynamic cluster configurations and varying computational loads across different nodes. The system must be capable of redistributing constraint evaluation tasks when nodes join or leave the cluster, while maintaining consistency in constraint satisfaction across all distributed components. Additionally, the scalability framework addresses the challenge of constraint communication overhead in large-scale deployments, utilizing compression algorithms and smart caching strategies to minimize the bandwidth requirements for constraint synchronization. The distributed architecture also incorporates adaptive load balancing mechanisms that can dynamically adjust the distribution of constraint evaluation tasks based on the computational capacity and current workload of individual cluster nodes, ensuring optimal resource utilization while maintaining system responsiveness and constraint integrity.

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BENCHMARKING AND PERFORMANCE ANALYSIS

Comprehensive benchmarking against existing methods reveals the trade-offs between interpretability gains and computational costs, incorporating evaluation methodologies that assess both predictive performance and constraint satisfaction across diverse application domains (Ge, K. *et al.*, 2024). Experimental results across multiple datasets demonstrate that per-class monotonicity constraints can improve model interpretability without significant accuracy degradation in most scenarios, with performance evaluation conducted using standard machine learning benchmarks and domain-specific datasets that reflect real-world application requirements. The computational overhead analysis considers multiple factors, including dataset size, constraint density, feature dimensionality, and class count, providing comprehensive insights into the scalability characteristics of the proposed methodology.

Performance analysis indicates that the proposed methodology performs particularly well in domains with inherent monotonic relationships, such as credit scoring, medical diagnosis, and risk assessment, where domain knowledge provides clear guidance on expected feature-outcome relationships. In these applications, the interpretability gains often justify the additional computational cost, especially when regulatory compliance or domain expert validation is required, demonstrating the practical value of constraint-based approaches in high-stakes decision-making scenarios. The evaluation framework incorporates metrics that assess both traditional predictive performance measures and constraint-specific evaluation criteria that quantify the degree of monotonicity preservation across different feature ranges and class combinations (Ke, G. *et al.*, 2017)

Comparison with post-hoc interpretability methods shows that built-in constraints provide more reliable and consistent feature relationships than external interpretation techniques, demonstrating superior stability and reliability in constraint enforcement. The constraint enforcement during training ensures that monotonic relationships are preserved throughout the model, rather than being approximated after training completion, providing stronger guarantees about model behavior in deployment scenarios. Cross-validation studies across multiple domains and datasets provide empirical evidence for the robustness and generalizability of the proposed approach, while ablation studies isolate the contributions of different algorithmic components to overall performance improvements.

The comprehensive evaluation framework extends beyond traditional accuracy metrics to include interpretability-specific measures that quantify the degree of constraint satisfaction and the stability of monotonic relationships across different data subsets and perturbations. This includes analysis of constraint robustness under various forms of data noise and adversarial attacks, ensuring that the interpretability guarantees remain valid even when the model is deployed in challenging real-world environments. The benchmarking study also investigates the long-term stability of constraint enforcement as models are updated with new training data, addressing the critical question of whether monotonic relationships remain consistent as the underlying data distribution evolves over time. Furthermore, the evaluation includes user studies with domain experts to assess the practical utility of the constraint-based interpretations, measuring whether the monotonic relationships discovered by the algorithm align with expert knowledge and provide actionable insights for decision-making processes.

Table 3: Performance Comparison Results (Ge, K. *et al.*, 2024; Ke, G. *et al.*, 2017)

Domain	Traditional XGBoost Accuracy	Constrained XGBoost Accuracy	Constraint Satisfaction Rate	Interpretability Score
Credit Scoring	High	High	Excellent	Superior
Medical Diagnosis	High	High	Excellent	Superior
Risk Assessment	High	Medium-High	Good	High
Image Classification	High	Medium	Fair	Medium
Text Classification	Medium-High	Medium	Good	Medium

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CONCLUSION

The development of monotonicity constraints for multiclass XGBoost represents a significant advancement in interpretable machine learning, successfully addressing the complex challenge of maintaining transparent feature-prediction relationships across multiple class outputs while preserving predictive performance. The constraint matrix framework enables flexible specification of class-specific monotonic relationships, providing domain experts with powerful tools to encode their knowledge directly into the learning process. The modified tree-building algorithm effectively balances accuracy and interpretability through constraint-aware splitting criteria that ensure global consistency across all binary classifiers in the one-vs-rest ensemble. The adaptive penalty-based loss function modifications demonstrate superior convergence properties while maintaining constraint satisfaction across diverse application domains. The distributed computing architecture proves scalable and fault-tolerant, supporting large-scale deployments without compromising constraint integrity or system reliability. The benchmarking results confirm that built-in constraints provide more reliable and consistent interpretability compared to post-hoc methods, particularly excelling in regulated industries where transparency is mandatory. The framework's ability to handle feature interactions and maintain constraint consistency across tree ensembles establishes a new standard for interpretable gradient boosting in multiclass scenarios. The practical applications in credit scoring, medical diagnosis, and risk assessment demonstrate the real-world value of constraint-based interpretability, enabling organizations to deploy machine learning systems that meet both performance and regulatory requirements. Future developments may extend these principles to other ensemble methods and explore automated constraint discovery techniques that can identify monotonic relationships directly from data patterns.

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