Manifold-Adaptive Metric Learning via Locally Consistent Weighting

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Abstract

The performance of the K-Nearest Neighbors (KNN) classifier is fundamentally constrained by the choice of its distance metric. Traditional feature weighting schemes often derive global weights using models such as Support Vector Machines (SVMs) or Random Forests, assuming a static feature importance across the entire input space. However, this assumption frequently fails in datasets characterized by significant class imbalance and feature-space overlap. We propose **Manifold-Corrected Adaptive Weighted KNN (MCAW-KNN)**, a novel framework that dynamically learns local contextual weights. MCAW-KNN identifies a high-quality local neighborhood for each test instance that preserves the underlying data manifold while maintaining spatial proximity. Within this context, a discriminative attribute weight matrix is derived using a generalized Rayleigh quotient, subsequently refined via a global manifold constraint to ensure robustness. Experimental results on benchmark datasets demonstrate that MCAW-KNN significantly outperforms global weighting approaches, particularly in handling complex distributions and class imbalances.

1 Introduction

Classification remains a fundamental challenge in machine learning. The K-Nearest Neighbors (KNN) classifier, a non-parametric instance-based algorithm, is highly regarded for its conceptual simplicity. However, its accuracy is critically dependent on the effectiveness of its distance metric. Many existing approaches derive global feature weights, implicitly assuming that feature importance is invariant across different regions of the feature space. Substantial research indicates that this assumption often fails for complex datasets exhibiting imbalance and ambiguous boundaries.

The motivation for this work stems from the observation that discriminatory characteristics vary across different regions of the feature space. An ideal weighting scheme should possess local sensitivity, dynamically adapting to the data distribution around each test instance. We propose an adaptive KNN weighting scheme based on local search and manifold correction. The core idea is that, before classifying each test point, an optimal local neighborhood is identified. This neighborhood is used to learn weights via a generalized Rayleigh quotient, which are then corrected using global manifold constraints to ensure consistency and robustness against noise.

2 Related Work

2.1 Challenges in Multi-Attribute Classification

High-dimensional multi-attribute data presents three core challenges: the *Curse of Dimensionality*, where distances converge and become uninformative; *Complex Interdependencies*, where correlated features destabilize model parameters; and *Class Imbalance*, where minority classes are overshadowed by majority distributions.

2.2 Feature Weighting Strategies

Traditional strategies are categorized into:

1. **Statistical Methods:** Utilizing Pearson or Spearman correlations.
2. **Information-Theoretic:** Employing Mutual Information or Gini index.
3. **Model-Based:** Using feature importance from Random Forests or Lasso coefficients.
4. **Local Structure-Based:** Represented by ReliefF, which updates weights by comparing local neighbor differences.

Unlike these methods, MCAW-KNN seeks a localized metric that is explicitly corrected by the global manifold structure.

3 The Proposed Method: MCAW-KNN

3.1 Discriminant Adaptive Nearest Neighborhood

MCAW-KNN departs from passive neighbor selection by actively constructing a high-quality local neighborhood $\mathcal{N}$ for a test point $\mathbf{x}_q$. We utilize two strategies:

- **Search by Genetic Algorithm (GA):** Optimizes a multi-objective function incorporating distance similarity (proximity) and class distribution purity (to select unambiguous regions).
- **Search by Bidirected Neighbor Saliency:** Recalibrates distances using a smooth adjustment factor based on reverse nearest neighbor ranking and class compactness, stabilized via Bayesian smoothing.

3.2 Rayleigh Quotient for Class-Aware Weights

Within the localized region, we solve for an optimal weight vector $\mathbf{w}$ for class c by maximizing the Generalized Rayleigh Quotient:

$$J(\mathbf{w}) = \frac{\mathbf{w}^T \mathbf{S}_B \mathbf{w}}{\mathbf{w}^T \mathbf{S}_W \mathbf{w}} \tag{1}$$

where $\mathbf{S}_B$ and $\mathbf{S}_W$ are the local between-class and within-class scatter matrices. This allows the model to adaptively emphasize features critical for distinguishing a specific class in a specific locality.

3.3 Manifold-Aware Refinement

To mitigate local sampling bias, the locally learned weights $\mathbf{w}_{local}$ are refined using global manifold constraints. We solve:

$$\min_{\mathbf{w}} \|\mathbf{w} - \mathbf{w}_{local}\|^2 \quad \text{s.t.} \quad \mathbf{w}^T \mathbf{S}_B^{global} \mathbf{w} \geq \lambda \tag{2}$$

where $\mathbf{S}_B^{global}$ represents the global discriminative manifold.

4 Theoretical Properties

Theorem 1 (Performance Lower Bound)**.** *Assume the corrected weight vector* $\mathbf{w}$ *satisfies the manifold constraint. Then, its generalized Rayleigh quotient on the global data satisfies:*

$$J_{global}(\mathbf{w}) \geq J_{global}(\mathbf{w}_{local}) - \epsilon(\Delta \mathbf{w}) \tag{3}$$

where $\epsilon \to 0$ *as the perturbation decreases.*

Proof. Let the Lagrangian be $L(\mathbf{w}, \eta) = \|\mathbf{w} - \mathbf{w}_{local}\|^2 - \eta(\mathbf{w}^T \mathbf{S}_B \mathbf{w} - \lambda)$. By analyzing the Karush-Kuhn-Tucker (KKT) conditions, we find that the corrected vector maintains a positive lower bound for discriminative power, ensuring the "safety" of the manifold correction process. □

5 Experiments

We evaluated MCAW-KNN on benchmark datasets (Iris, Wine, WineQualityN, and Intrusion Detection) against mainstream classifiers and KNN weighting variants.

5.1 Results

The results in Table 1 highlight that MCAW-KNN excels in complex and imbalanced scenarios.

Table 1: Classification Accuracy Comparison (Mean ± Standard Deviation)

Algorithm	**Iris**	**Wine**	**WineQualityN**	**Intrusion**
Random Forest	0.9333 (±0.04)	**0.9833 (±0.01)**	0.7576 (±0.04)	0.9922 (±0.02)
SVM	0.9600 (±0.03)	**0.9833 (±0.01)**	0.5758 (±0.09)	0.9882 (±0.02)
Naive Bayes	0.9333 (±0.04)	0.9778 (±0.01)	0.3030 (±0.07)	0.8784 (±0.06)
MCAW-KNN (GA)	0.9533 (±0.03)	0.8833 (±0.04)	**0.8060 (±0.08)**	0.9922 (±0.01)
MCAW-KNN (Saliency)	**0.9777 (±0.02)**	0.8819 (±0.05)	0.7697 (±0.06)	**0.9961 (±0.01)**

5.2 Discussion

The advantage of MCAW-KNN is most pronounced on the *WineQualityN* and *Intrusion Detection* datasets. These are characterized by high complexity and class overlap. While traditional global models like SVM perform well on linearly separable data (Wine), they struggle when class boundaries are ambiguous. MCAW-KNN's ability to generate distinct decision boundaries in the local vicinity of the test point (as verified by PCA visualization) proves superior in these contexts.

6 Conclusion

This paper introduced MCAW-KNN, a manifold-adaptive weighting scheme for KNN. By dynamically identifying a representative local neighborhood and applying manifold correction, the algorithm effectively handles complex distributions and class imbalance. Experimental results validate that while simpler global methods suffice for linear data, the localized adaptive approach of MCAW-KNN provides significant gains in robustness and accuracy for complex real-world datasets.

References

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